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12-14 June 2007, at US Naval Academy, Annapolis, MD

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Leveraging Process Knowledge to Improve Modeling of Evaporation Rate Data for Agent Fate Wind Tunnels

Presented at
75th MORS Symposium
13 June 2007

Thomas A. Donnelly, Ph.D.
R&T Directorate, ECBC

DISCLAIMER: The findings presented in this briefing are not to be construed as an official
Department of the Army position unless so designated by other authorizing documents.

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Purpose of Talk

- Demonstrate how the modeling (regression analysis) of evaporation rate data can be improved by rescaling the variables based on knowledge of the process
- Describe how running the experimental design trials in specific randomized blocks – as compared to running the planned trials in a haphazard order – facilitates:
 - A sequential model building process
 - Identifying when running more trials adds little new information



Summary

- Rescaling the variables using knowledge of the physics reduces the complexity of the model required to adequately fit the data
 - Before rescaling, a 10-term quadratic model was needed
 - After rescaling, a 4-term linear model is all that is needed
- Extrapolated predictions for checkpoints within the 5-cm tunnel data validate “nearby” extrapolation with the physics-based linear model
- For the physics-based linear model “farther out” extrapolations are more plausible than those of the empirical model.
 - Note that these “farther out” conditions are beyond the practical range of the wind tunnels and that these predictions have not been validated.



Summary

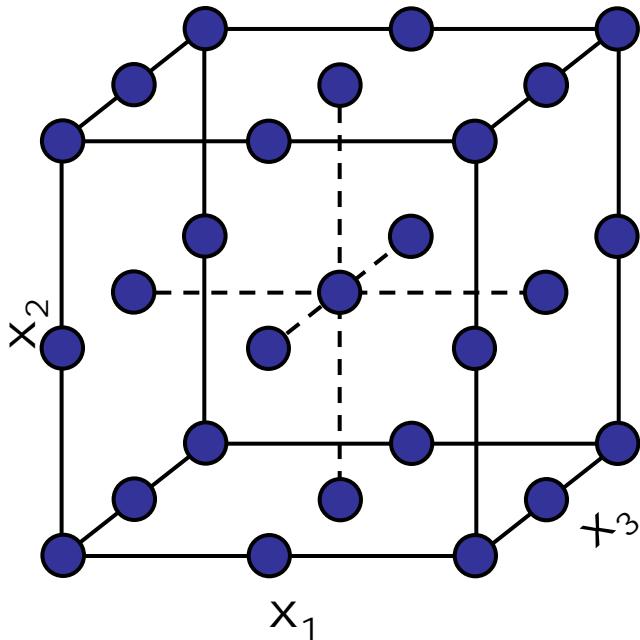
- Although the same level of reduction of the number of required trials seen for HD on glass may not hold true for other agents and/or substrates, results point to importance of running trials in a sequence of blocks that support increasingly complex models.
- Combining the data for the 5-cm and 10-cm tunnels shows that the “tunnel effect” - although statistically significant - is dwarfed by the effects of the Temperature, Wind Velocity and Drop Size which are 5X to 14X as large. For HD on glass, the behavior of the two tunnels appears quite similar.



Data for HD on Glass Came from Two Sources

- 5-cm ECBC tunnel data
 - 19 unique trials – with one observation for each – i.e. no replicates
- 10-cm Czech tunnel data
 - 13 unique trials with 34 observations – eight 2X, four 3X and one 6X
- In both cases the original plan called for the running of a “validation design” - 27 unique trials making up the $3 \times 3 \times 3$ full-factorial design

3 X 3 X 3 Full-Factorial Design and Empirical Model Terms It Can Support

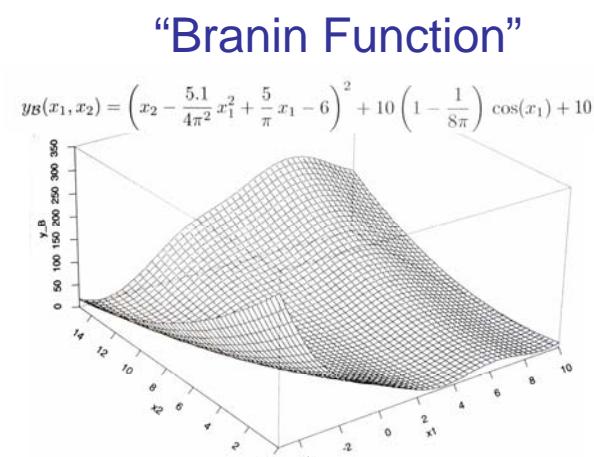
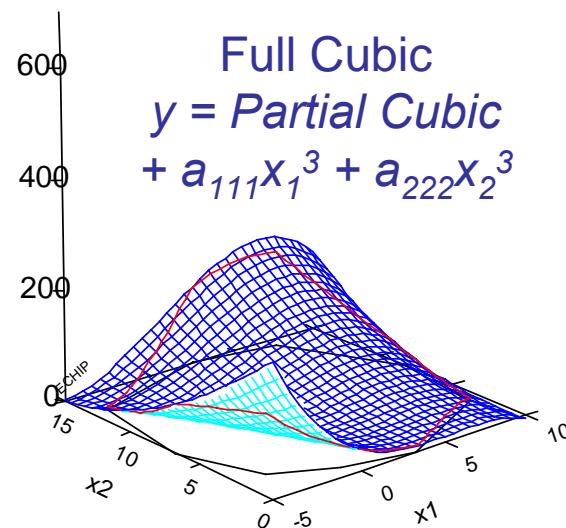
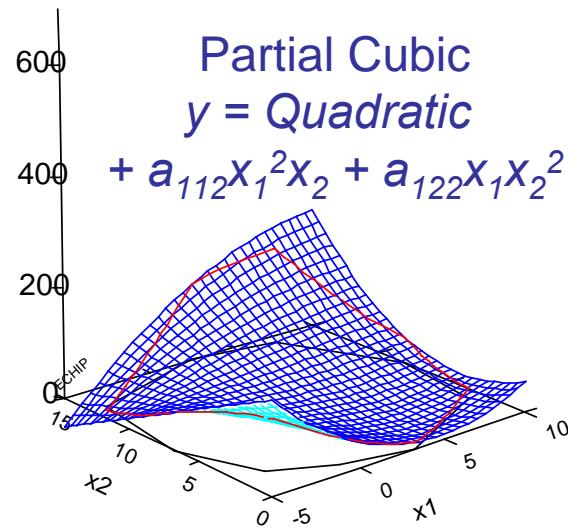
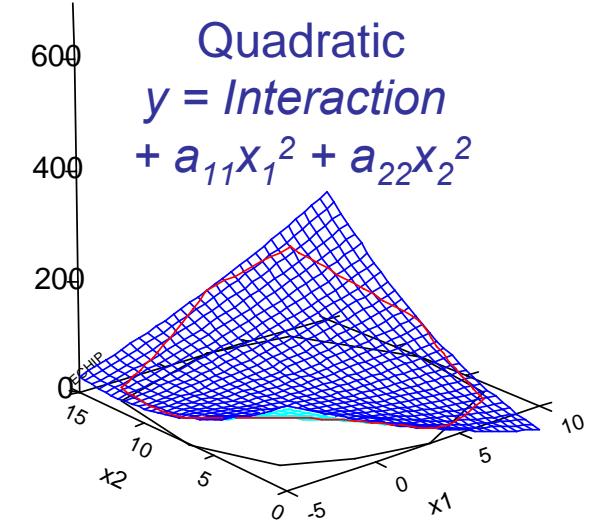
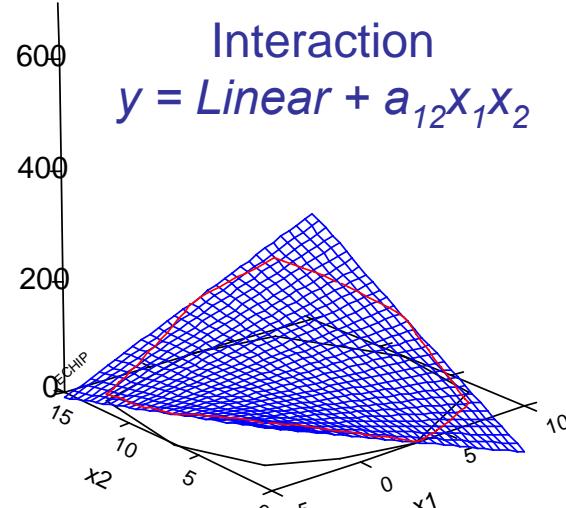
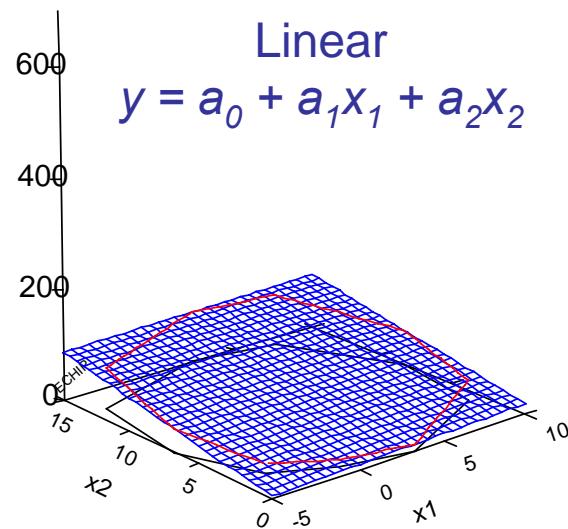


$$\begin{aligned}
 y = & a_0 + a_1 x_1 + a_2 x_2 + a_3 x_3 \\
 & + a_{12} x_1 x_2 + a_{13} x_1 x_3 + a_{23} x_2 x_3 \\
 & + a_{11} x_1^2 + a_{22} x_2^2 + a_{33} x_3^2 \\
 & + a_{123} x_1 x_2 x_3 \\
 & + a_{112} x_1^2 x_2 + a_{122} x_1 x_2^2 + a_{113} x_1^2 x_3 \\
 & + a_{133} x_1 x_3^2 + a_{223} x_2^2 x_3 + a_{233} x_2 x_3^2
 \end{aligned}$$

constant + linear
 + 2-way interactions
 + curvature terms
 + 3-way interaction
 + partial cubic terms

Because this design does not have 4 levels/variable, it cannot be used to fit full cubic terms such as $a_{111}x_1^3$, $a_{222}x_2^3$ and $a_{333}x_3^3$.

Comparing Surfaces for Increasingly Complex Polynomials Fit to Data from the Branin Function

FIGURE C.1. The Branin function on $[-5, 10] \times [0, 15]$

Of these models, the *full cubic* best approximates the Branin function, but still cannot represent the ripples visible on edges of the last plot.

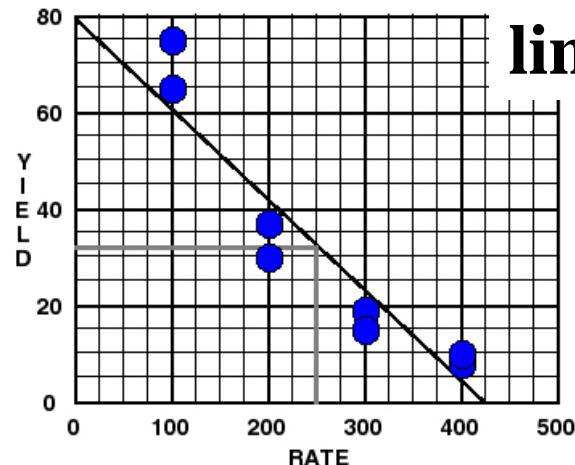


Data Transformations – Why Do Them?

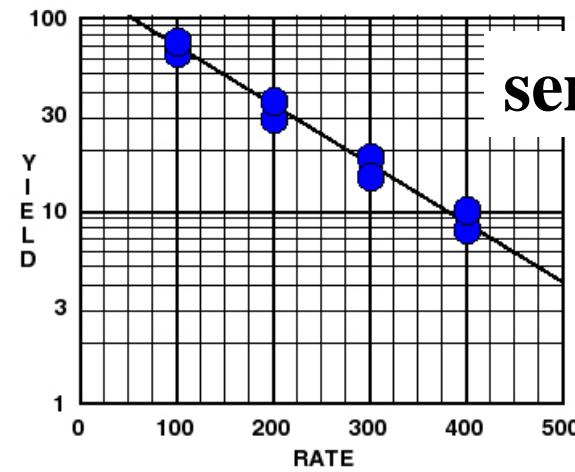
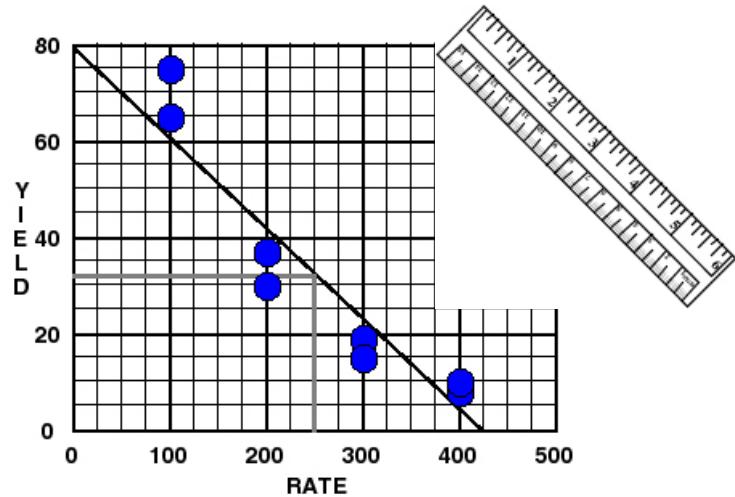
- Remedy for lack of fit
- Plot predictions will not violate physical limits
 - e.g. "# of Counts" not negative;
YIELD not $> 100\%$
- Make model more robust
- Make error more uniform across design region
 - (also called "stabilizing the variance")
 - Transformations change the scale of the response to make it more nearly conform to the usual regression assumptions, the most important of which are that the data are independent and *follow a normal distribution with a constant variance*.



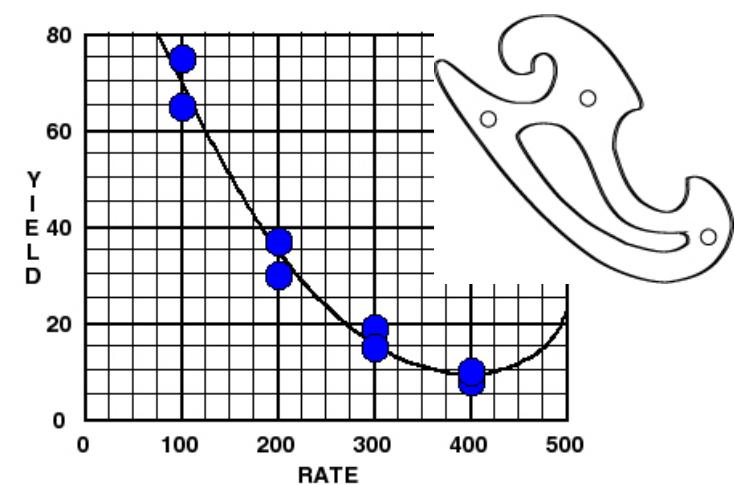
Two Remedies for Lack-of-Fit Fancier *Graph Paper* or Fancier *Curve*



linear



semi-log

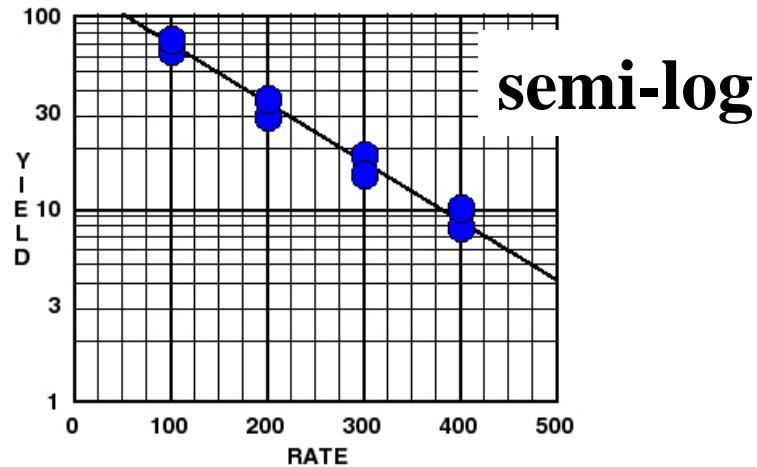


Does not require additional trials.

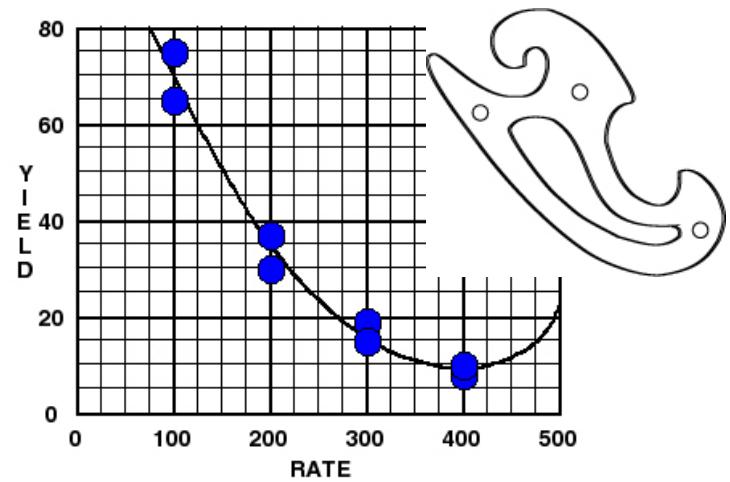
Usually requires additional trials.



Model Predictions are Virtually Same *within the Range of the Control Variable Settings (100 to 400)*



At Rate = 500
Predicted Yield is 4



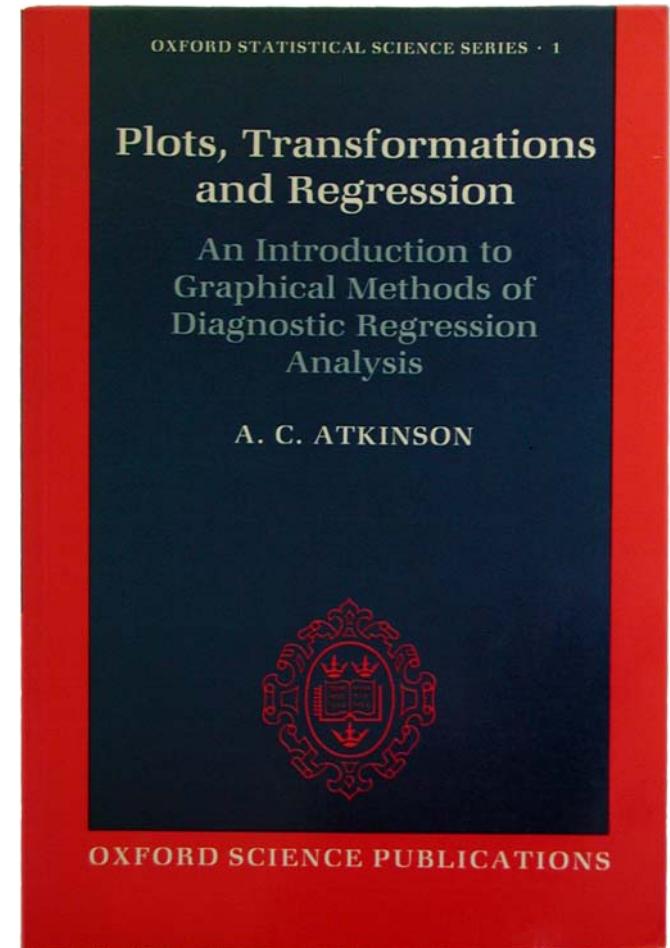
At Rate = 500
Predicted Yield is 22

Which prediction is more suspect? Why?



Have a *Reason* to Use a Transformation- DO NOT "Brute Force" Eliminate Lack-of-Fit

- Consult a book like 
- Check publications in your field to see how others present the same kind of data.
- Consult your local statistical expert.

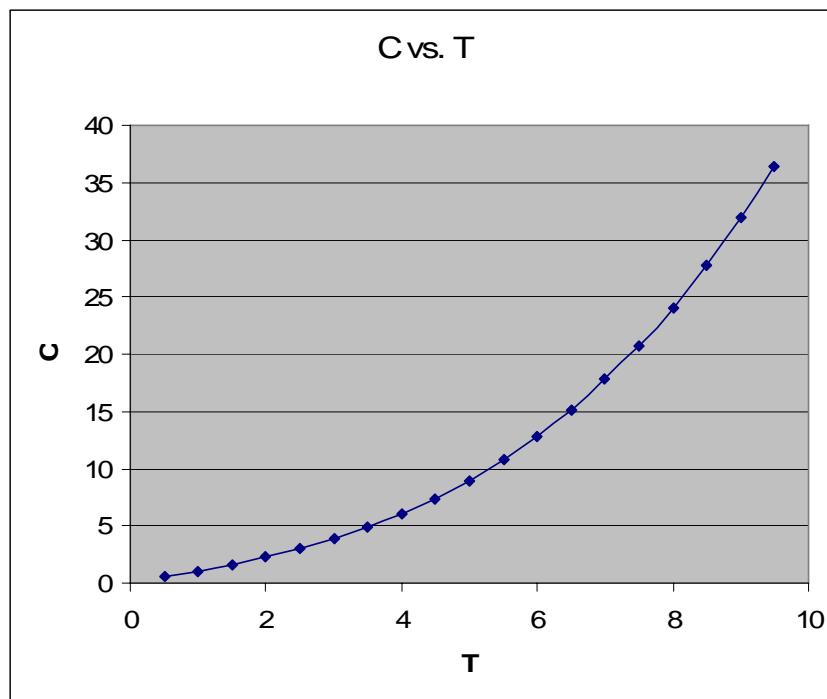




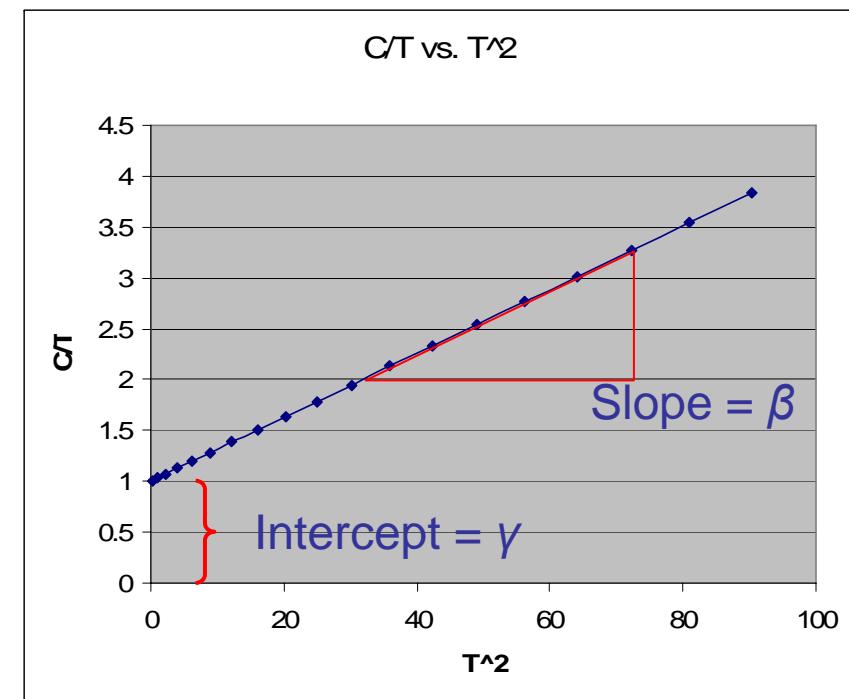
Example of How Rescaling Makes the Analysis Easier

Specific Heat of Metals for $T < 10^{\circ}\text{K}$

$$C = \gamma T + \beta T^3$$



$$C/T = \gamma + \beta T^2$$





What Knowledge Did We Use to Choose Variable Scaling?

- Evaporation rate and temperature have an Arrhenius relationship where Evap_Rate is proportional to $e^{(-1/kT)}$ which leads to the scaling choices of taking
 - the \log_{10} of the response, Evaporation Rate, (\log_e could have been used) and
 - the inverse of the control variable Temperature (in $^{\circ}\text{K}$)
- From Prof. J. Danberg via M. Miller - evaporation rate is proportional to the cube-root of the Wind Velocity
- Believing that evaporation rate was dependent on the area of the drop led to assumption that response should be proportional to square-root of the Drop Size.
 - Recently T. D'Onofrio pointed out that drop size is really a volume and therefore the calculated area of the drops is proportional to $(\text{Drop Size})^{2/3}$. It will be shown that reanalysis of the data using this new scaling makes for very minor changes in predictions and no altering of original conclusions.



Comparison of 10-term Quadratic and 4-term Linear Models

$$\begin{aligned}\log_{10}(y) = & a_0 + a_1x_1 + a_2x_2 + a_3x_3 \\ & + a_{12}x_1x_2 + a_{13}x_1x_3 + a_{23}x_2x_3 \\ & + a_{11}x_1^2 + a_{22}x_2^2 + a_{33}x_3^2\end{aligned}$$

constant + linear
+ 2-way interactions
+ curvature terms

The quadratic model can support many shapes – including; mountain, valley, ridge, saddle and plane.

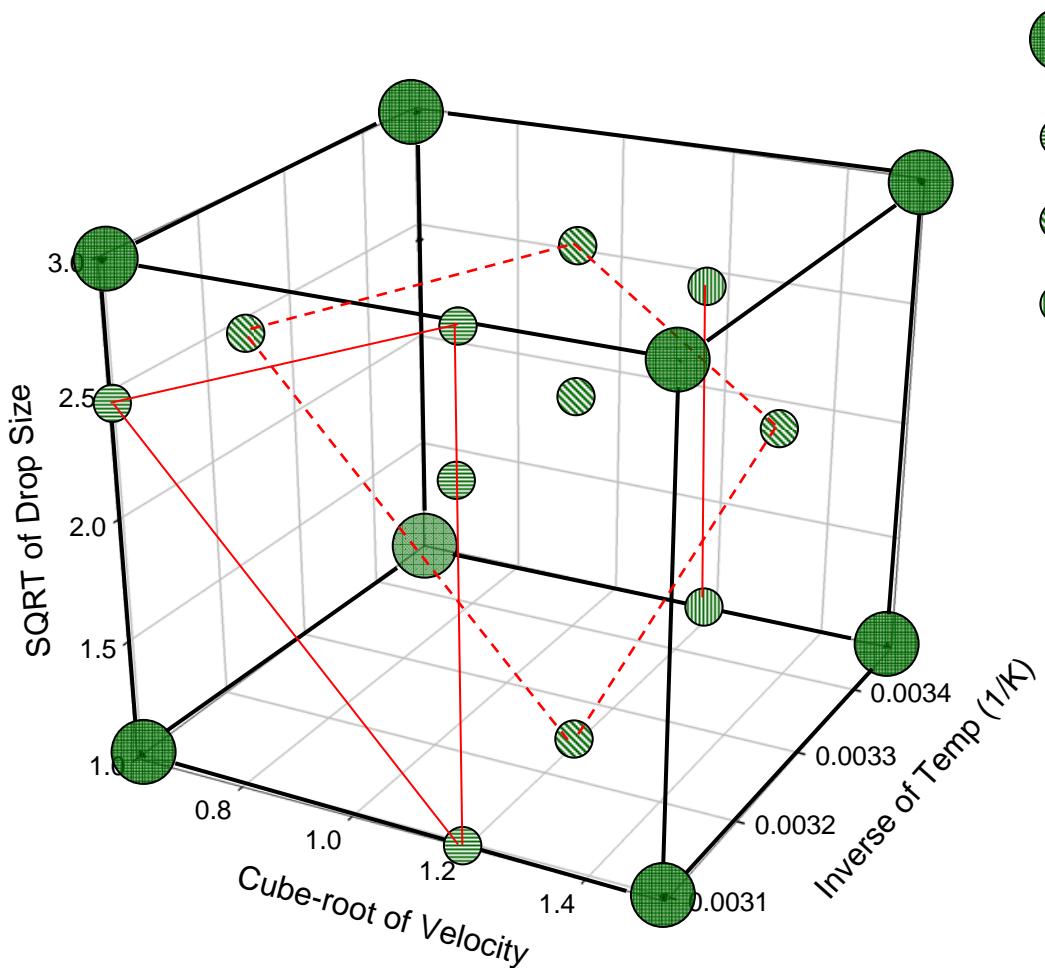
$$\begin{aligned}\log_{10}(y) = & A_0 + A_1X_1 + A_2X_2 + A_3X_3 \\ \text{and } X_1 = & (x_1)^{-1}, X_2 = (x_2)^{1/2}, X_3 = (x_3)^{1/3}\end{aligned}$$

constant + linear terms
sample exponents used
to “linearize” model

The linear model can only support a plane.



Locations of the 19 Unique Trial Settings for the 5-cm Tunnel



- 8 extreme (corner) points
- 4 internal points on hi T (low $1/T$) front face
- 5 internal points on intermediate T slice
- 2 internal points on low T (hi $1/T$) back face

Red lines indicate the area on each slice of $1/T$ enclosed by the shaded (internal) points

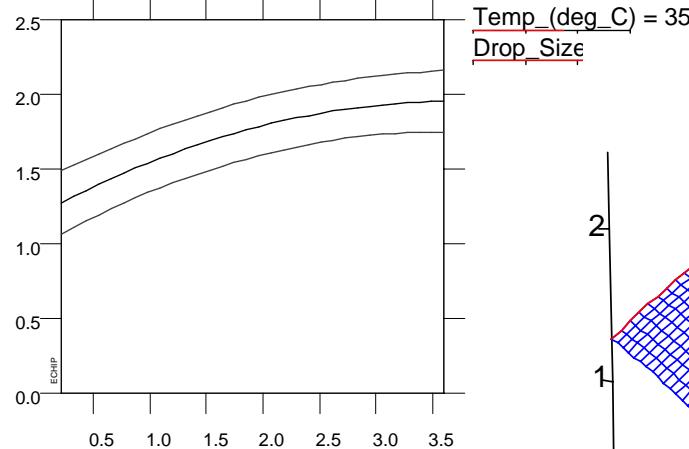


Comments on 5-cm Tunnel Analyses

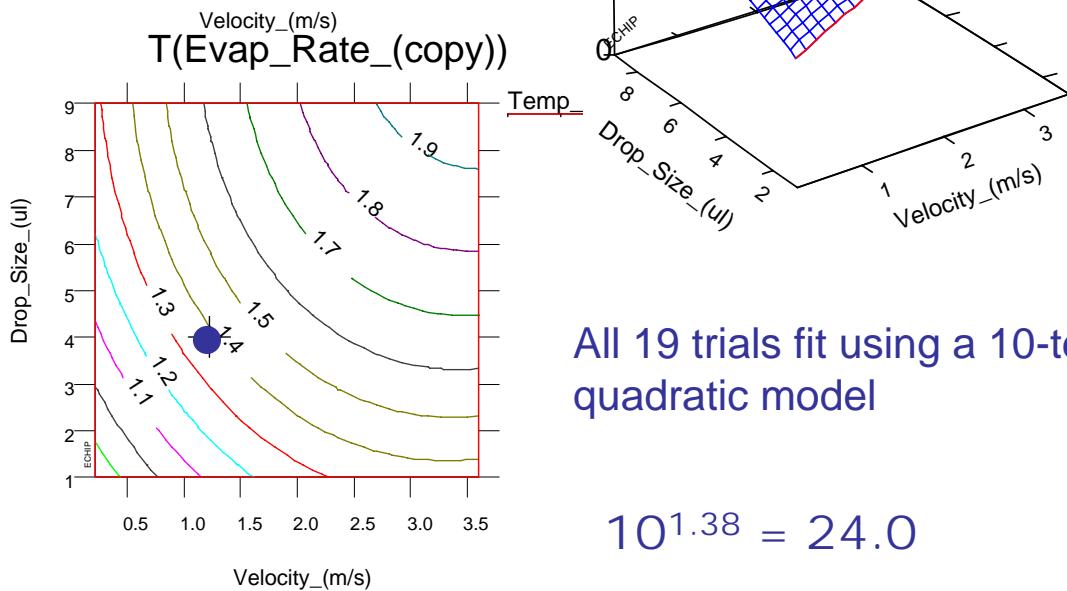
- Good news: Physics-based linearized model fits well - has slightly smaller model error (residual std. dev.) and higher Adjusted-R² than empirical model
- Better news: *Interpolated* model predictions based on fitting data at 8 corner design points are validated by data at locations of 11 interior design trials - which were not used in fitting model
- Even better news: Reversing the situation, the *extrapolated* model predictions based on fitting data at 11 interior points are validated by data at 8 corners - which were not used in fitting model
- Maybe best news: As few as 4 corner points + 1 center point are needed for the 80% solution...

Interpolation with Empirical Quadratic Model (Response Transformed to \log_{10} Scale)

T(Evap_Rate_(copy))



T(Evap_Rate_(copy))



All 19 trials fit using a 10-term quadratic model

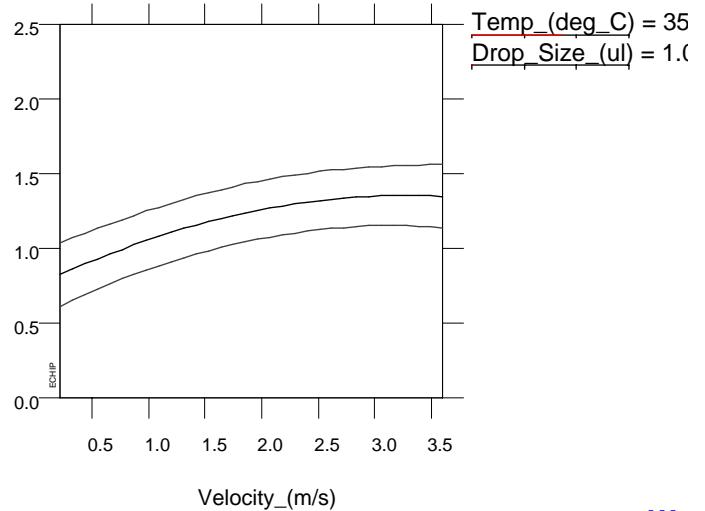
$$10^{1.38} = 24.0$$

| | | | |
|---------------|---------------|-----------------|----------------------|
| Velocity=1.23 | Value 1.38 | Plot SD 0.04 | Predicted SD 0.09 |
|---------------|---------------|-----------------|----------------------|

Temp_(deg_C) = 35.0

1-D, 2-D & 3-D plots of Evap_Rate vs. Velocity and Drop_Size with \log_{10} transformation “applied”

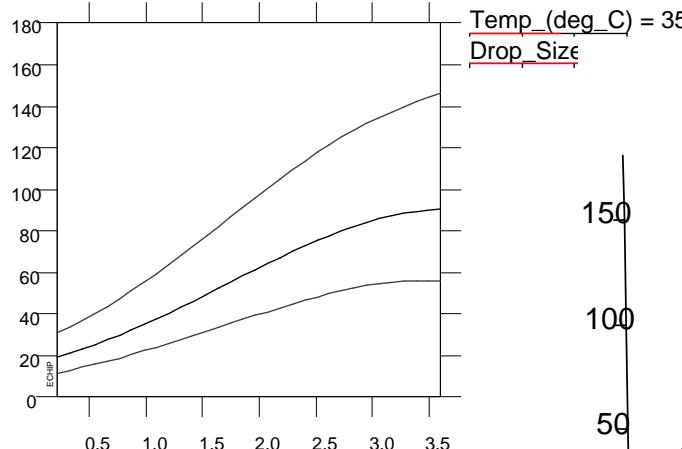
T(Evap_Rate_(copy))





Interpolation with Empirical Model (Response Transformed Back to Original Scale)

Evap_Rate_(copy)

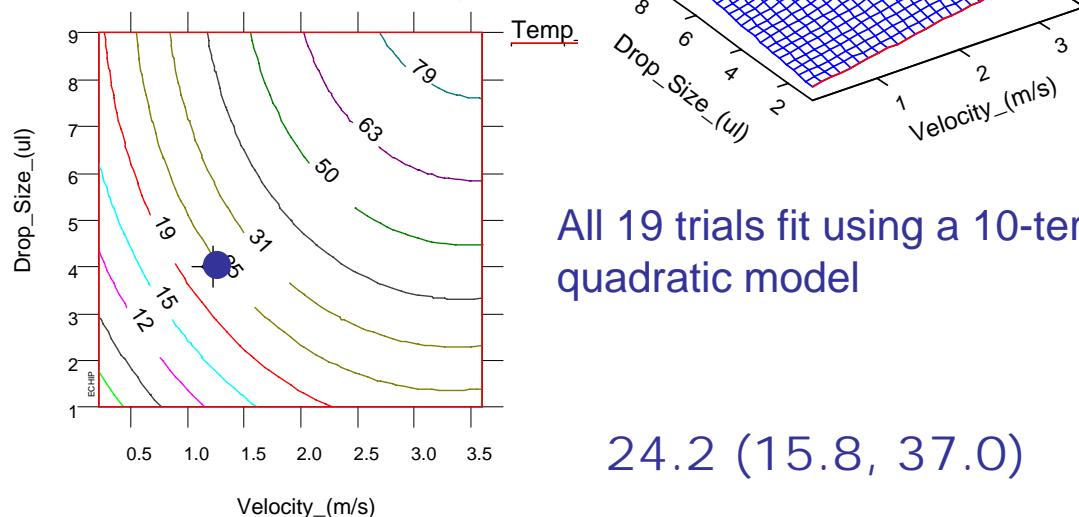


Evap_Rate_(copy)



1-D, 2-D & 3-D plots of Evap_Rate vs. Velocity and Drop_Size with \log_{10} transformation “undone”

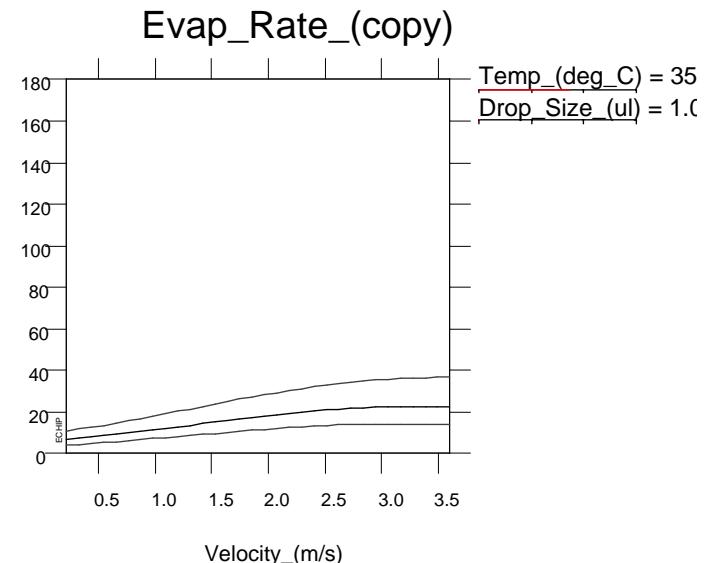
Evap_Rate_(copy)



All 19 trials fit using a 10-term quadratic model

24.2 (15.8, 37.0)

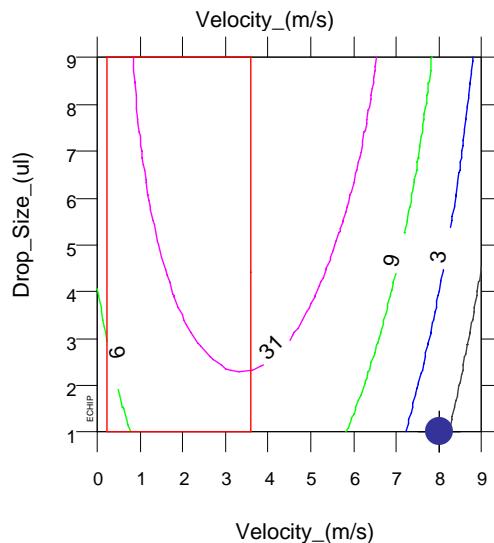
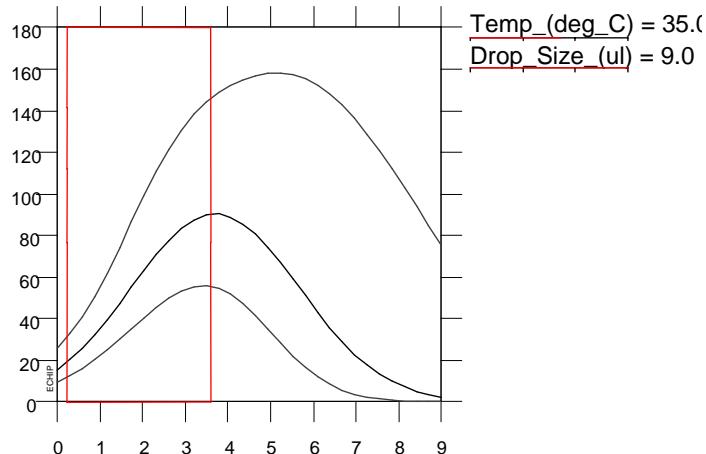
| | | |
|---------------|-----------------|------------------|
| Velocity=1.23 | Value 24.21 | Drop_Siz=4.00 |
| | Low Limit 15.83 | High Limit 37.03 |





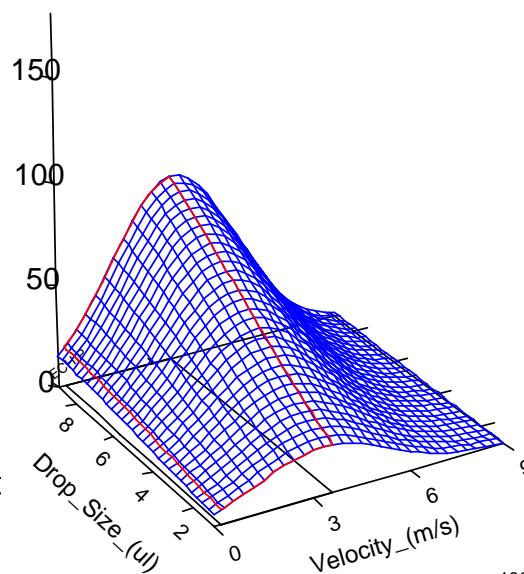
Extrapolation with Empirical Model (Response Transformed Back to Original Scale)

Evap_Rate_(copy)



| | |
|---------------|----------------|
| Velocity=8.00 | Drop_Siz=1.00 |
| Value 1.33 | Low Limit 0.10 |

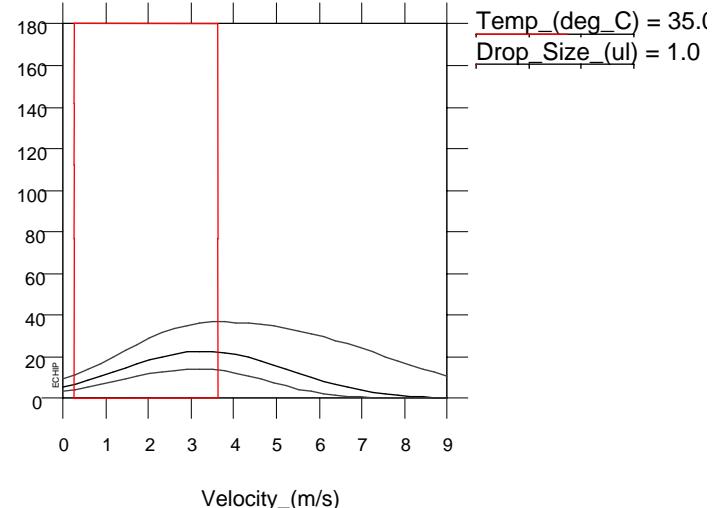
Evap_Rate_(copy)



All 19 trials fit using a 10-term quadratic model

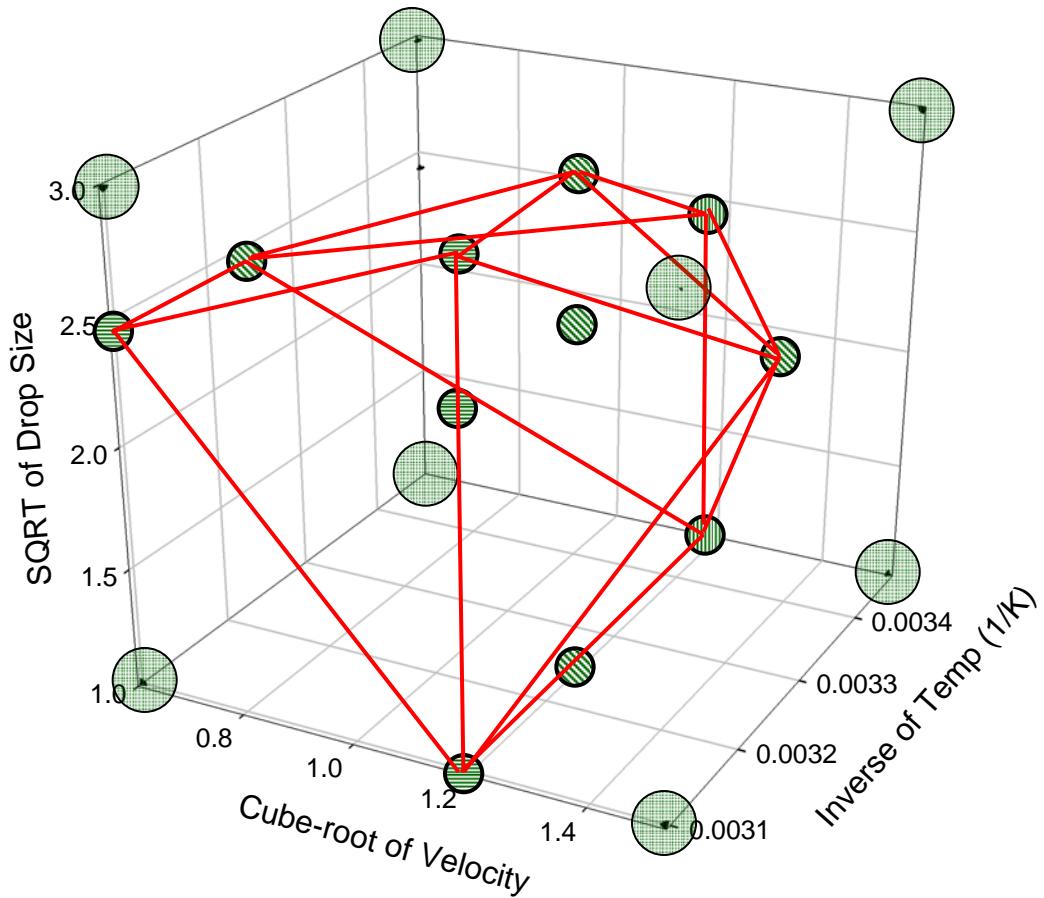
Predicted Evap_Rate
At 8 m/s = 1.3 (0.1, 17.1)

Evap_Rate_(copy)





Volume Enclosed by the 11 Unique Interior Trials for the 5-cm Tunnel



The red polyhedral shape results from “shrink wrapping” the 11 non-corner design trials for the 5-cm tunnel.

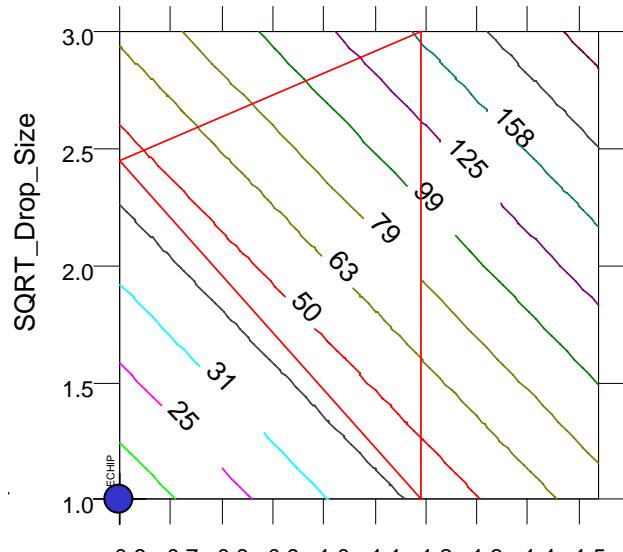
Predictions at the 8 corners of the design region made using a model fit to these 11 points are *extrapolated* predictions.



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Predictions on Raw and Transformed Scales at Location of the Poorest Performing Extrapolated Checkpoint

Evap_Rate_(copy)



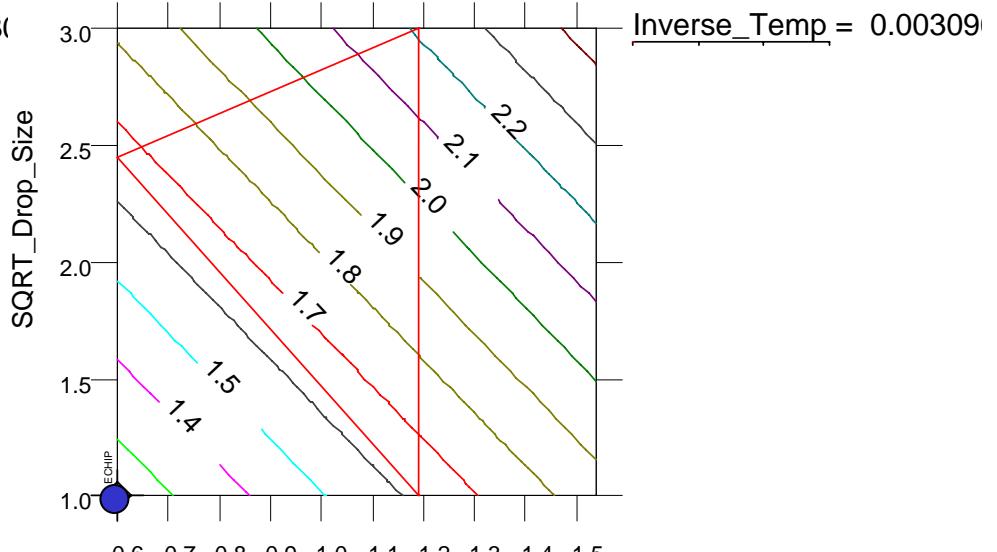
Cube-root_of_Vel

| Cube-roo=0.60 | Value | Low Limit | High Limit |
|---------------|-------|-----------|------------|
| | 16.88 | 10.10 | 28.20 |

Predicted value is 16.88 on raw scale
with 95% Prediction Limits of 10.10 to 28.20
Observed value was **21.6** on raw scale

Observed $\log_{10}(21.6) = 1.33$

T(Evap_Rate_(copy))



Cube-root_of_Vel

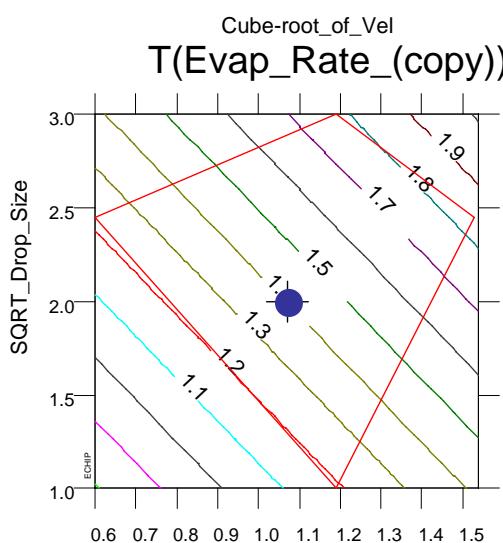
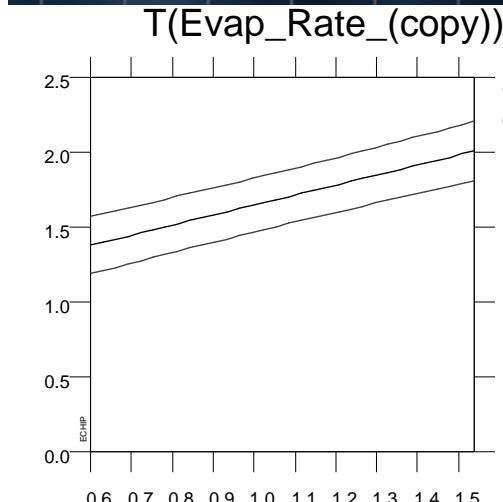
| Cube-roo=0.60 | Value | Plot SD | SQRT_Dro=1.00 | Predicted SD |
|---------------|-------|---------|---------------|--------------|
| | 1.23 | 0.07 | 1.00 | 0.11 |

Predicted value is 1.23 on log10 scale
Within one Predicted SD (0.11) of the
Observed value of **1.33** on log10 scale

Predicted $10^{1.23} = 16.98$

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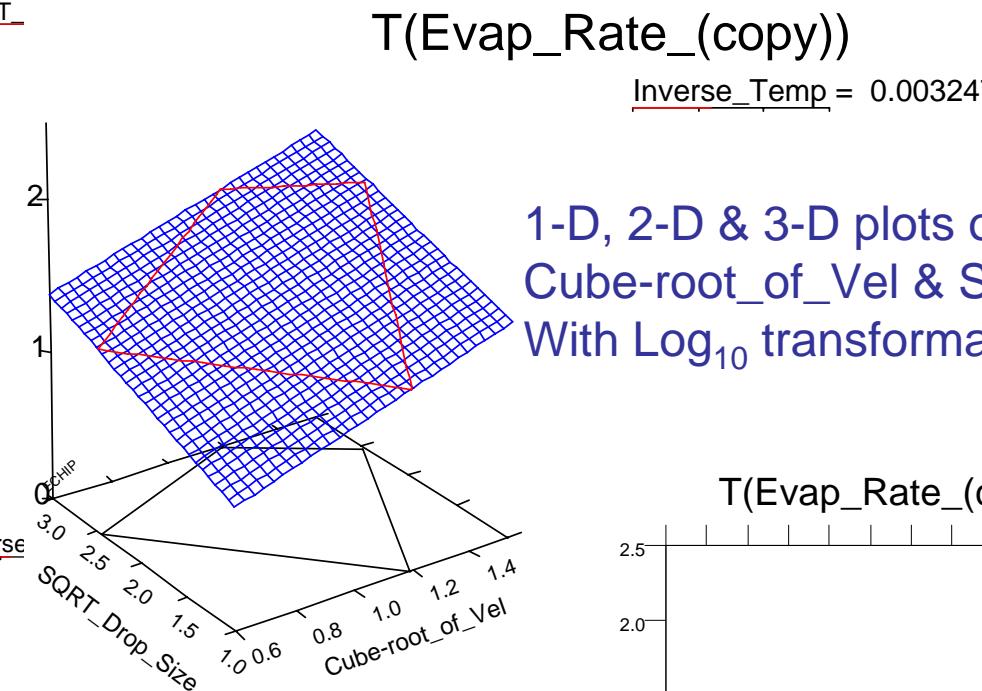
Interpolation w/Physics-Based Linear Model (Response Transformed to \log_{10} Scale)



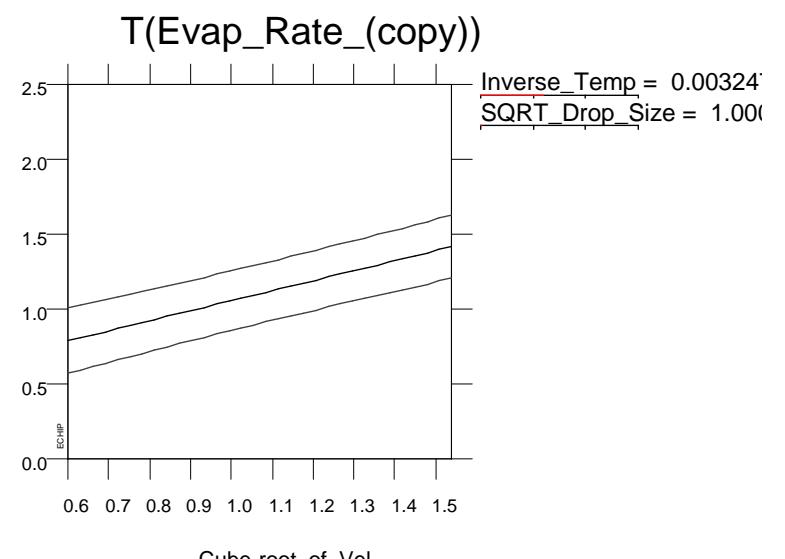
| Cube-root=1.07 | Value 1.40 | Plot SD 0.03 | SQRT_Dro=2.00 | Predicted SD 0.08 |
|----------------|------------|--------------|---------------|-------------------|
| | | | | |

$$10^{1.40} = 25.1$$

11 interior trials fit using a 4-term linear model that is physics based



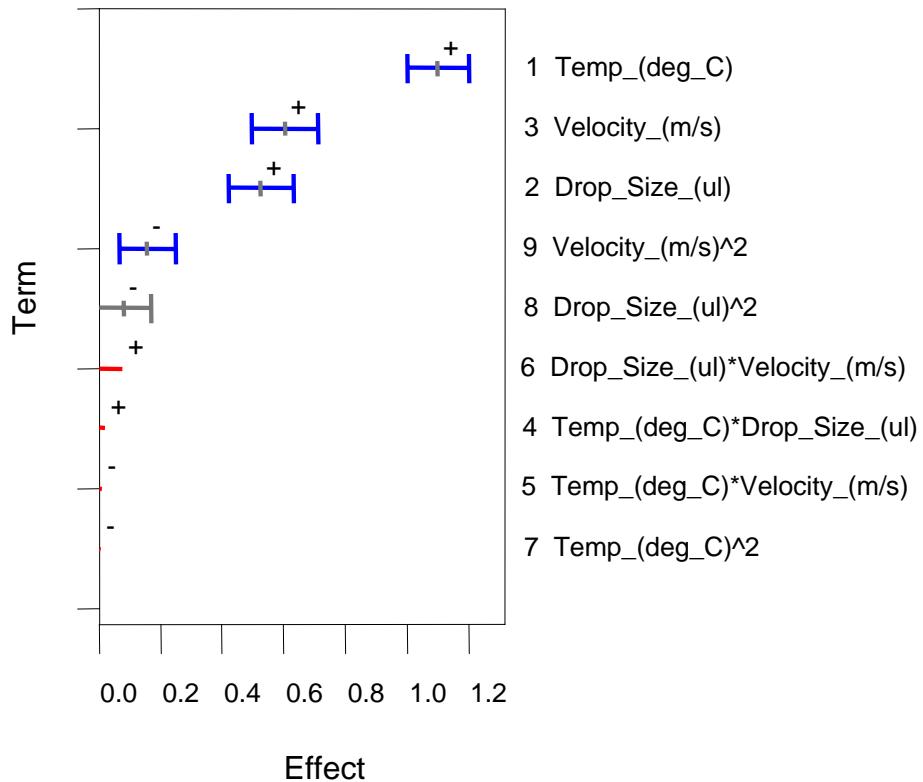
1-D, 2-D & 3-D plots of Evap_Rate vs. Cube-root_of_Vel & SQRT_Drop_Size With \log_{10} transformation “applied”



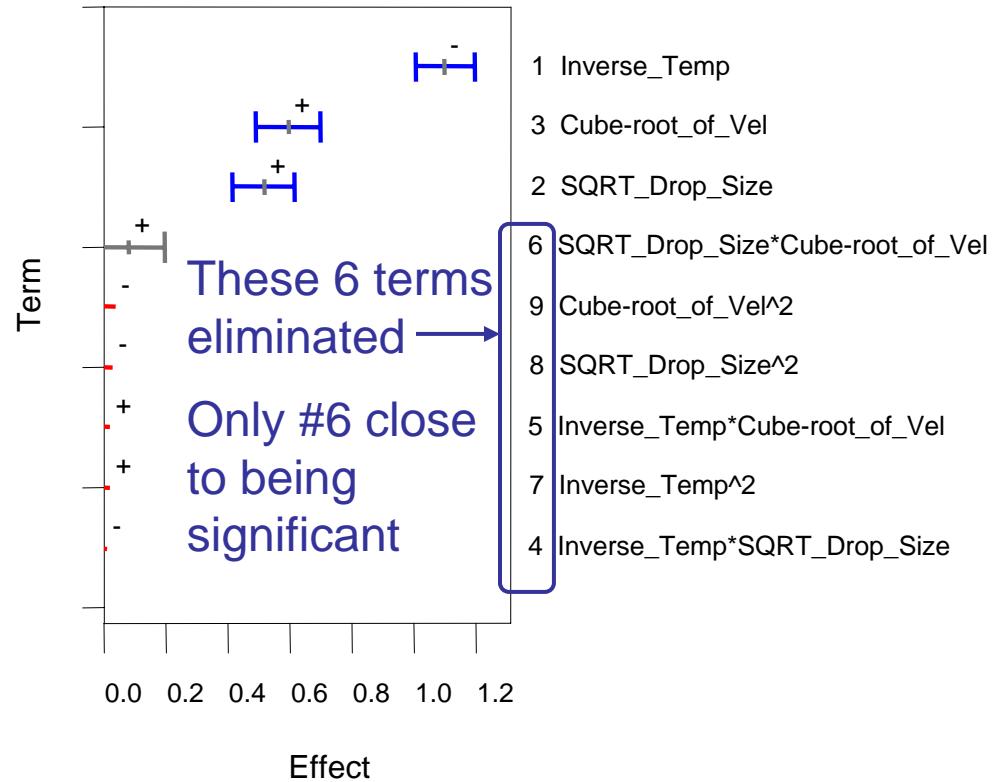


Comparison of Ranked Effect Estimates for 10-term Quadratic Models Fit to Unscaled and Scaled Control Variables

Pareto Effects for $\log_{10}(\text{Evap_Rate})$



Pareto Effects for $\log_{10}(\text{Evap_Rate})$



An Effect is the Change in the Response, $\log_{10}(\text{Evap_Rate})$,
Resulting from Changing a Variable Setting from Low to High



Comparison of Model Error Estimates

Quadratic Model without rescaling of control variables

N trials = 19
 N terms = 10
 Residual DF = 9
 Residual SD = 0.0782

Cross val RMS = 0.1061

R Squared = 0.992
 Adj R Squared = 0.983

Linear Model with rescaling of control variables

N trials = 19
 N terms = 4
 Residual DF = 15
 Residual SD = 0.0700 ← Smaller

Cross val RMS = 0.0778 ← Smaller

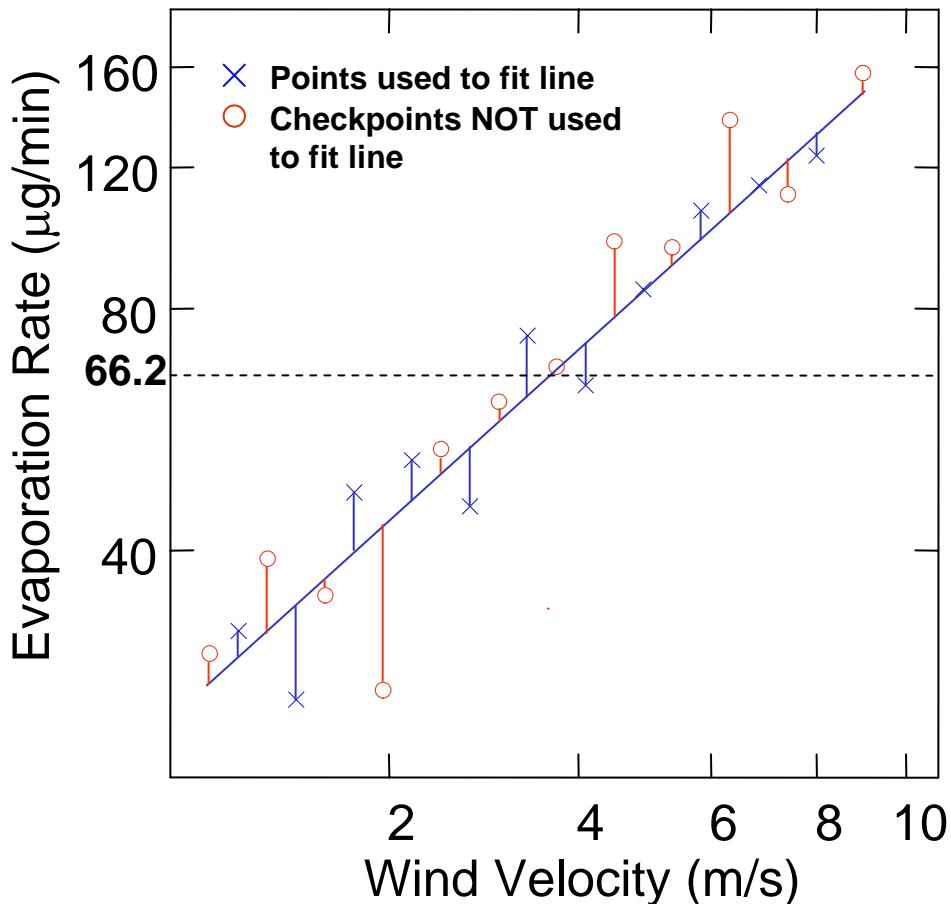
R Squared = 0.989
 Adj R Squared = 0.986 ← Higher

Results are similar but slightly
better for the 4-term linear model



Comparing Residual SD, Checkpoint RMS and Raw SD for a Single Control Variable

(NOTE: Real Data NOT Used in this Comparison)



N trials = 11

N terms = 2

Residual DF = 9

Residual SD = 0.0655

(Model error)

N checkpoints = 12

Checkpoint RMS = 0.0808

(Prediction error)

Raw SD = 0.2245

(Error about mean of data for 11 trials used to fit)

Graph paper used has \log_{10} vertical scale and cube-root horizontal scale.



Comparing Residual SD, Checkpoint RMS and Raw SD

- When Residual SD ~ Checkpoint RMS then model error is comparable to prediction error
 - Residual SD calculated from the differences between the observed and fitted (predicted) values
 - Checkpoint RMS calculated from the differences between the observed and predicted values - BUT the observed values were NOT used to fit the model used to make the predictions
- Ideally both Residual SD and Checkpoint RMS should be “far” from Raw SD (SD about the Mean of the data)
 - There is no statistical test for how far apart they should be, but for the closer case – the fitting of the 11 internal points - the Raw SD (0.4923) is 6 times larger than both the Checkpoint RMS (0.0765) and the Residual SD (0.0785)



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Comparison of Model Error and Checkpoint Error for 8 Corners and 11 Internal Points

Fit of 8 Corner Points and Use 11 Internal as Checkpoints

N trials = 8
N terms = 4
Residual DF = 4
Residual SD = 0.0633
Raw SD = 0.7332

N checkpoints = 11
Checkpoint RMS = 0.0816
Cross val RMS = 0.0895

R Squared = 0.996
Adj R Squared = 0.993

Fit of 11 Internal Points and Use 8 Corners as Checkpoints

N trials = 11
N terms = 4
Residual DF = 7
Residual SD = 0.0785
Raw SD = 0.4923

N checkpoints = 8
Checkpoint RMS = 0.0765
Cross val RMS = 0.1067

R Squared = 0.982
Adj R Squared = 0.975

Residual SD and Checkpoint RMS Values Agree Well

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Comparison of Checkpoint RMS for $V^{1/3}$ term (left) vs. $V^{2/3}$ term (right) Fitting 8 Corners w/11 Internal Checkpoints

Fit of 8 Corner Points and Use 11 Internal as Checkpoints

N trials = 8
N terms = 4
Residual DF = 4
Residual SD = 0.0633
Raw SD = 0.7332

N checkpoints = 11
Checkpoint RMS = 0.0816
Cross val RMS = 0.0895

R Squared = 0.996
Adj R Squared = 0.993

Fit of 8 Corner Points and Use 11 Internal as Checkpoints

N trials = 8
N terms = 4
Residual DF = 4
Residual SD = 0.0633
Raw SD = 0.7332

N checkpoints = 11
Checkpoint RMS = 0.1117
Cross val RMS = 0.0895

R Squared = 0.996
Adj R Squared = 0.993

Checkpoint RMS Better with $V^{1/3}$ than with $V^{2/3}$

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Comparison of Checkpoint RMS for DS^{1/2} term (left) vs. DS^{2/3} term (right) Fitting 11 Internal w/8 Corner Checkpoints

Fit of 11 Internal Points and Use 8 Corners as Checkpoints

N trials = 11
N terms = 4
Residual DF = 7
Residual SD = 0.0785
Raw SD = 0.4923

N checkpoints = 8
Checkpoint RMS = 0.0765
Cross val RMS = 0.1067

R Squared = 0.982
Adj R Squared = 0.975

Fit of 11 Internal Points and Use 8 Corners as Checkpoints

N trials = 11
N terms = 4
Residual DF = 7
Residual SD = 0.0776
Raw SD = 0.4923

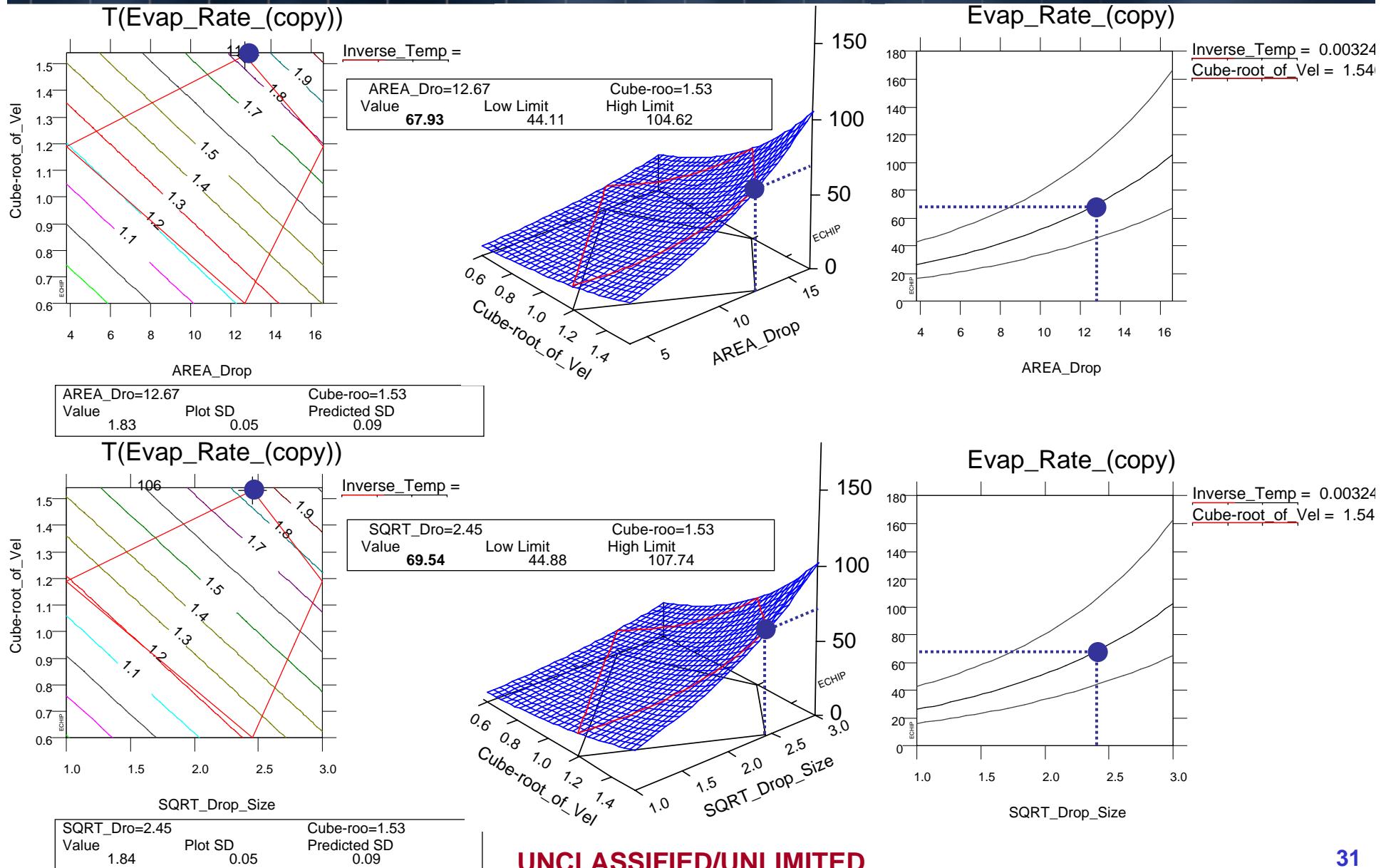
N checkpoints = 8
Checkpoint RMS = 0.0857
Cross val RMS = 0.1062

R Squared = 0.983
Adj R Squared = 0.975

Checkpoint RMS Better with DS^{1/2} than with DS^{2/3}

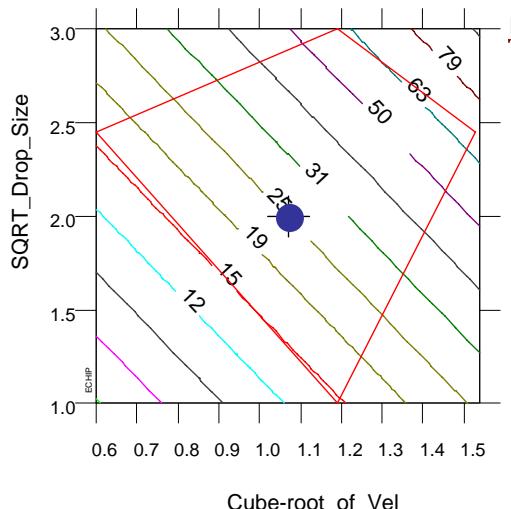
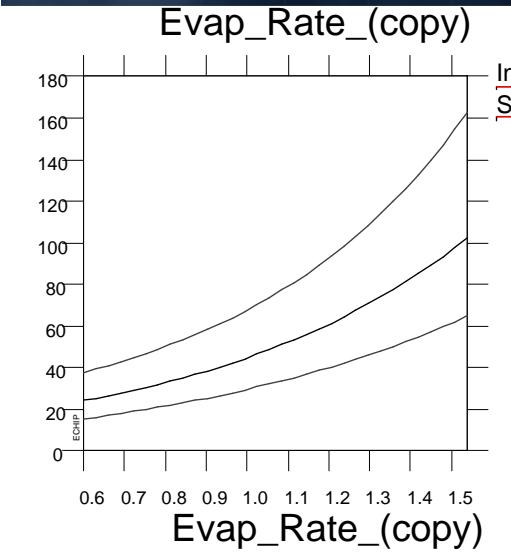
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Compare Predictions for Models Using AREA_Drop vs. SQRT_Drop_Size

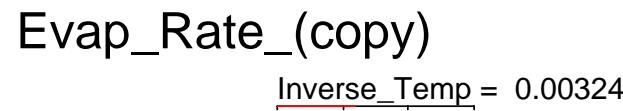




Interpolation w/Physics-Based Linear Model (Response Transformed Back to Original Scale)



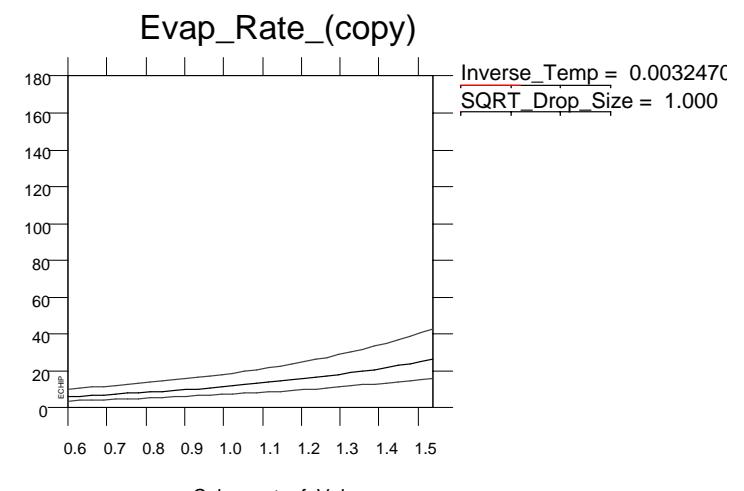
| Cube-root=1.07 | Value | SQRT_Dro=2.00 |
|----------------|-------|----------------------------------|
| | 25.25 | Low Limit 16.97 High Limit 37.58 |



1-D, 2-D & 3-D plots of Evap_Rate vs. Cube-root_of_Vel & SQRT_Drop_Size with \log_{10} transformation “undone”

11 interior trials fit using a 4-term linear model that is physics based

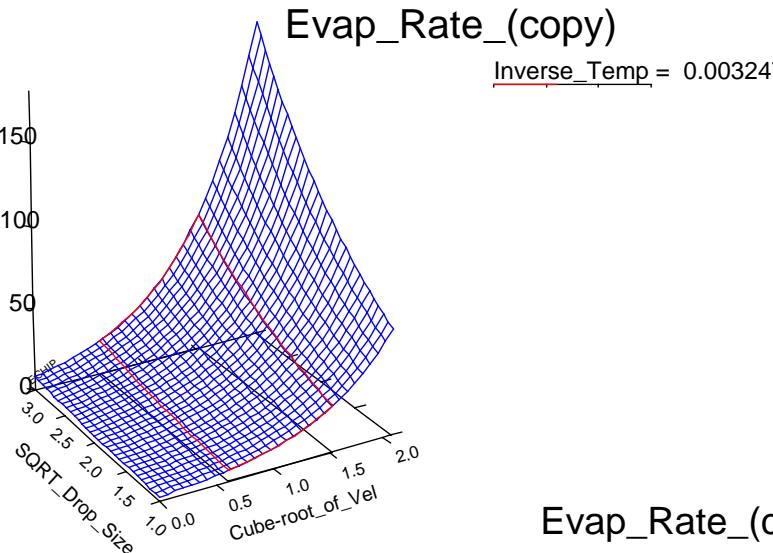
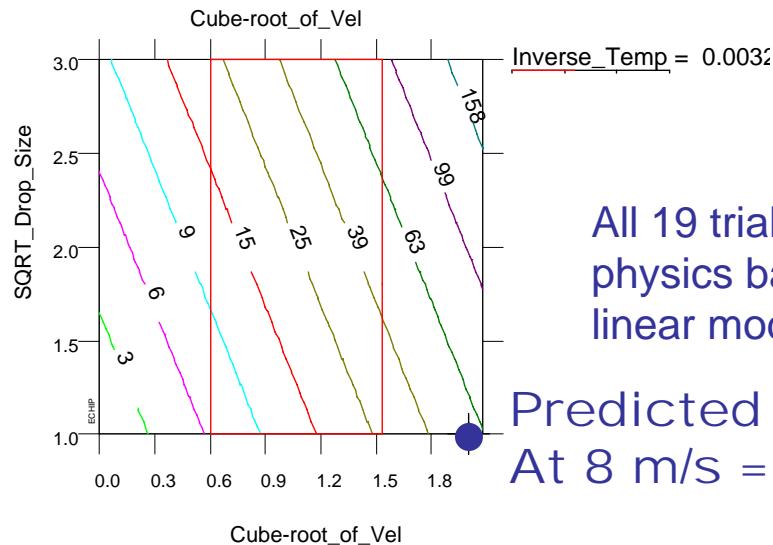
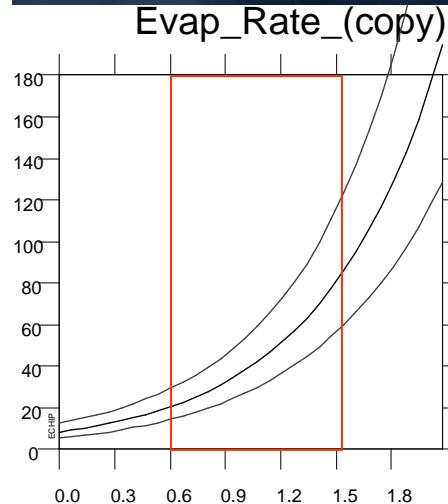
25.3 (17.0, 37.6)



— Cube-root_of_Vel
- - - Limits



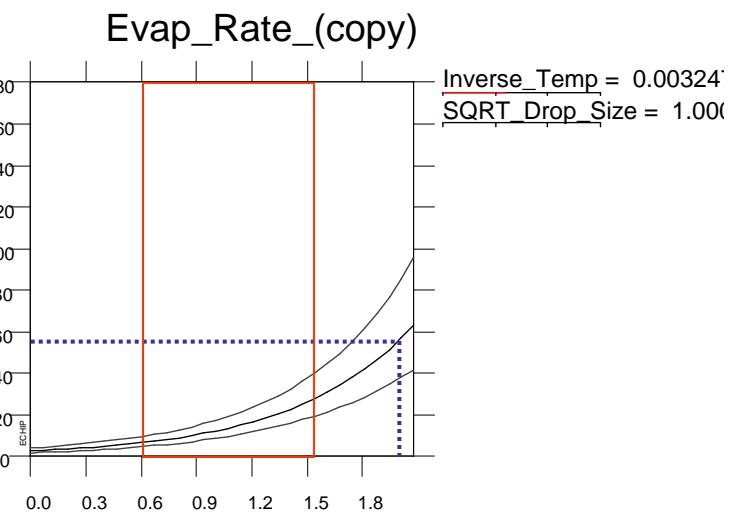
Extrapolation with Physics-Based Model (Response Transformed Back to Original Scale)



All 19 trials fit using a physics based 4-term linear model

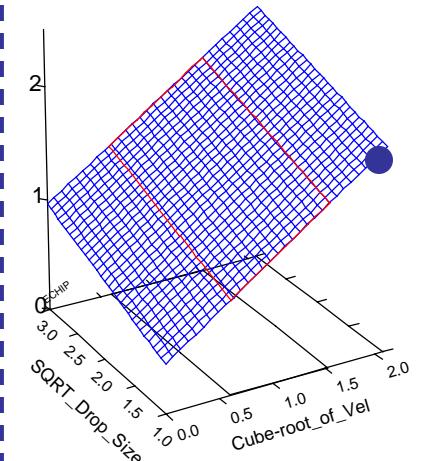
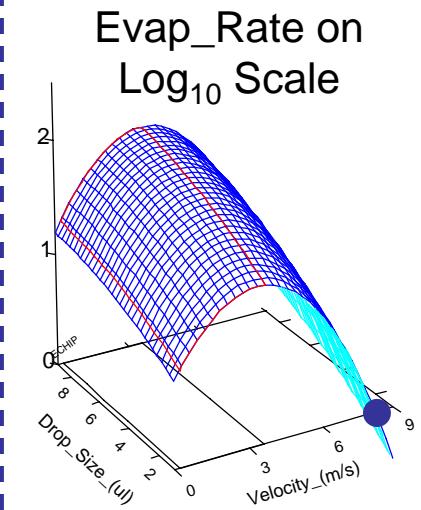
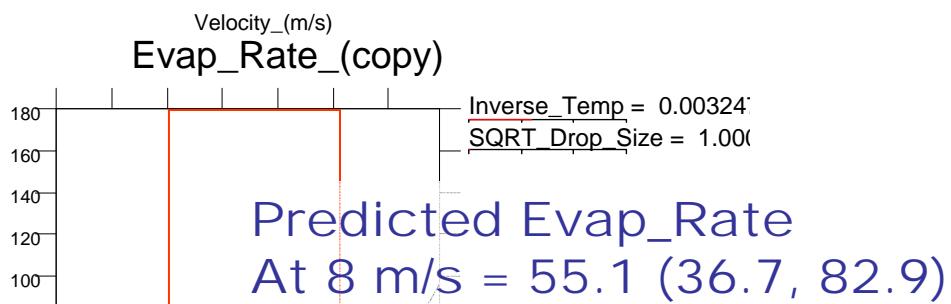
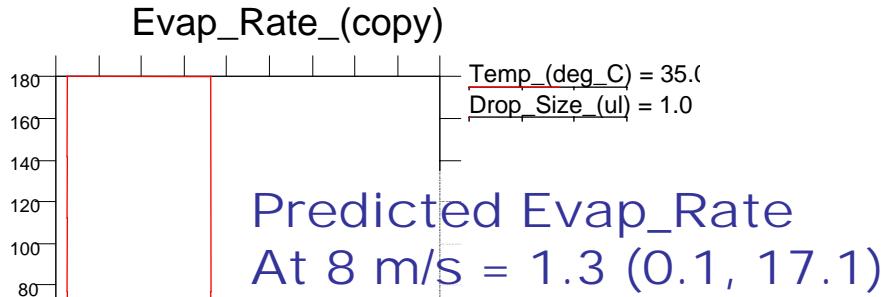
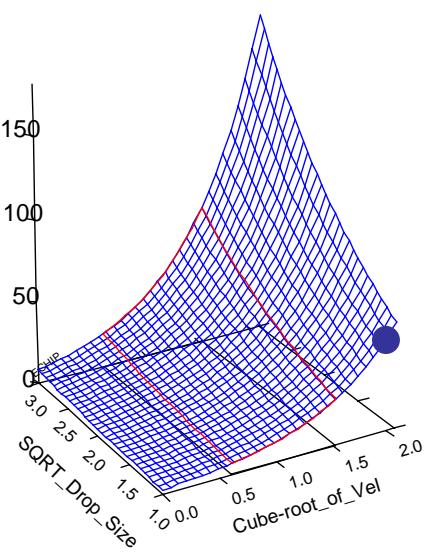
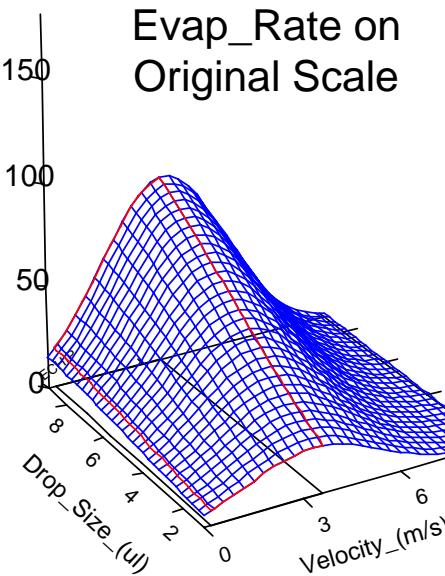
Predicted Evap_Rate
At 8 m/s = 55.1 (36.7, 82.9)

| | | |
|----------------------------------|--------------------|--------------------------------------|
| Cube-root=2.00 Value 55.11 | Low Limit 36.66 | SQRT_Dro=1.00 High Limit 82.85 |
|----------------------------------|--------------------|--------------------------------------|



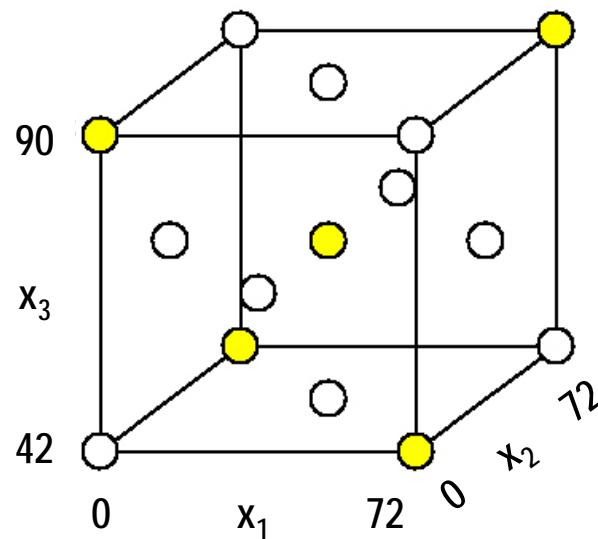
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Compare Extrapolations for Empirical (Quadratic) & Physics-Based (Linear) Models (Response Transformed Back to Original Scale)



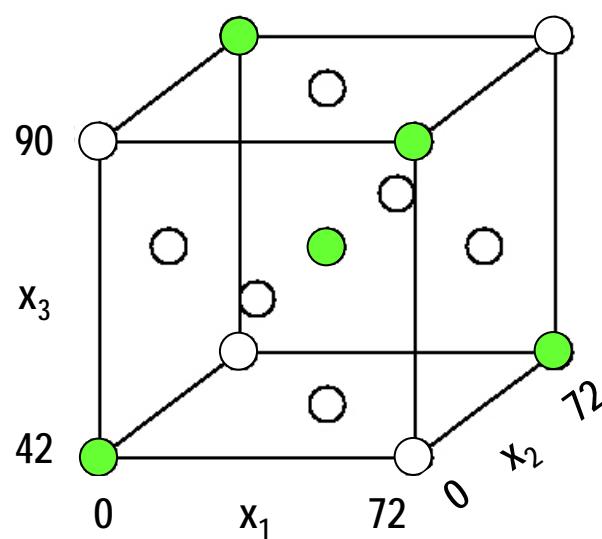


Sequentially Run Trials in Blocks

Block 1

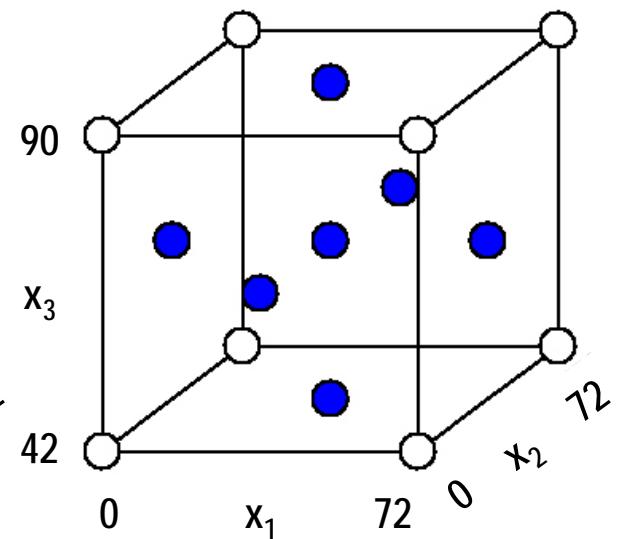
$$y = a_0 + a_1x_1 + a_2x_2 + a_3x_3$$

Linear model is supported by any of the three Blocks

Block 2

$$y = a_0 + a_1x_1 + a_2x_2 + a_3x_3$$

Interaction model is supported by combining first two Blocks

Block 3

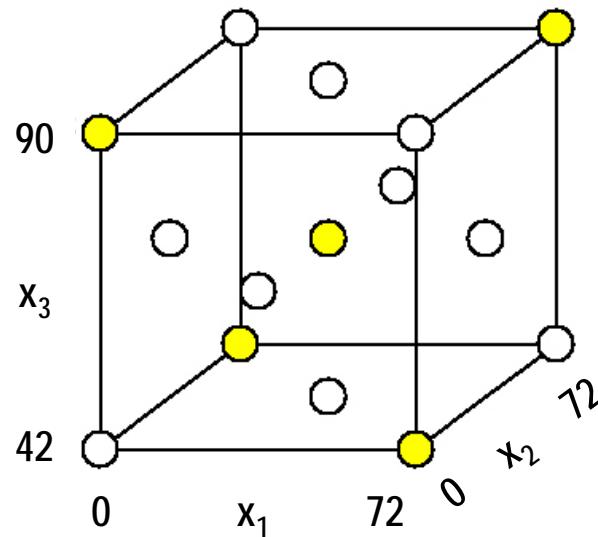
$$y = a_0 + a_1x_1 + a_2x_2 + a_3x_3 + a_{12}x_1x_2 + a_{13}x_1x_3 + a_{23}x_2x_3 + a_{11}x_1^2 + a_{22}x_2^2 + a_{33}x_3^2$$

Quadratic model requires all three Blocks to be supported

Blocking is used to prevent correlations between design variables and sources of variation such as unknown variables (e.g. blocks run weeks apart) or differences among groups of trials (e.g. each block associated with a unique “lot” of raw material)



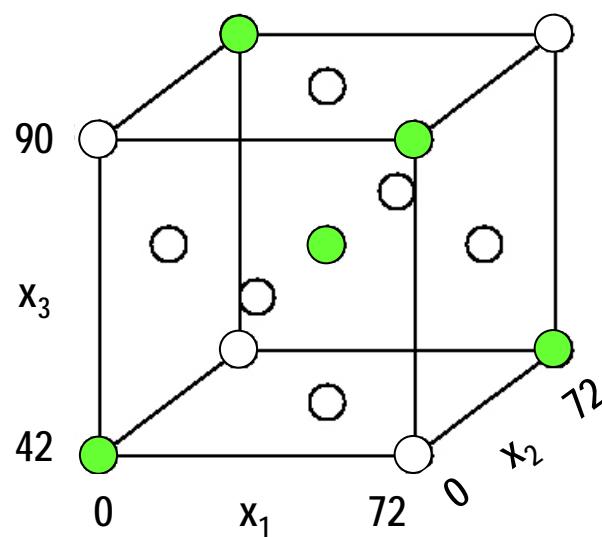
Sequentially Run Trials in Blocks

Block 1

$$y = a_0 + a_1x_1 + a_2x_2 + a_3x_3$$

Run this block 1st to

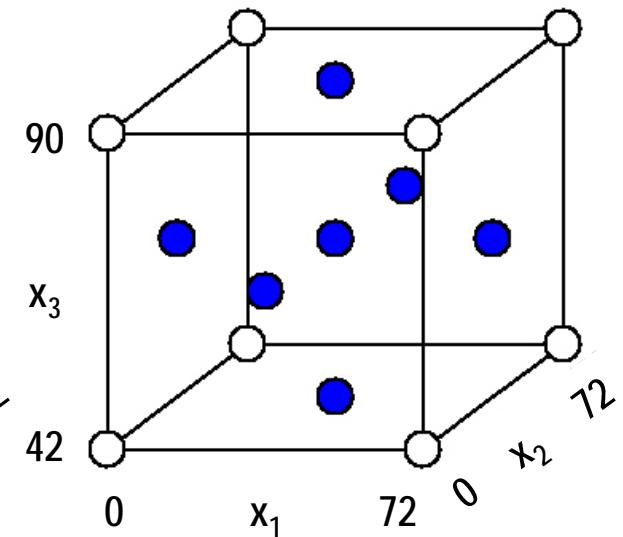
- (i) estimate the main effects
- (ii) use center point to check for curvature.

Block 2

$$y = a_0 + a_1x_1 + a_2x_2 + a_3x_3$$
$$+ a_{12}x_1x_2 + a_{13}x_1x_3 + a_{23}x_2x_3$$

Run this block 2nd to

- (i) repeat main effects estimate,
- (ii) check if process has shifted
- (iii) add interaction effects to model if needed.

Block 3

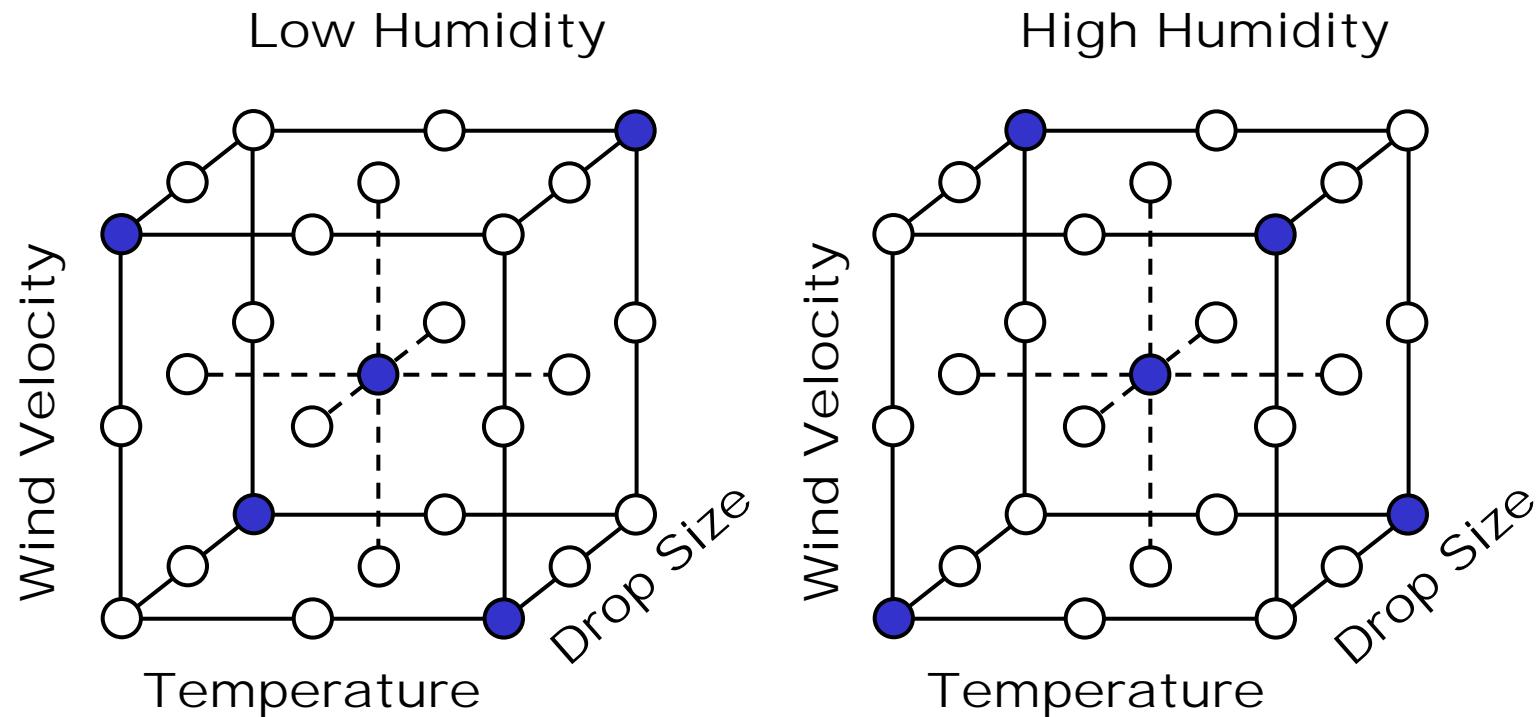
$$y = a_0 + a_1x_1 + a_2x_2 + a_3x_3$$
$$+ a_{12}x_1x_2 + a_{13}x_1x_3 + a_{23}x_2x_3$$
$$+ a_{11}x_1^2 + a_{22}x_2^2 + a_{33}x_3^2$$

Run this block 3rd to

- (i) repeat main effects estimate,
- (ii) check if process has shifted
- (iii) add curvature effects to model if needed.



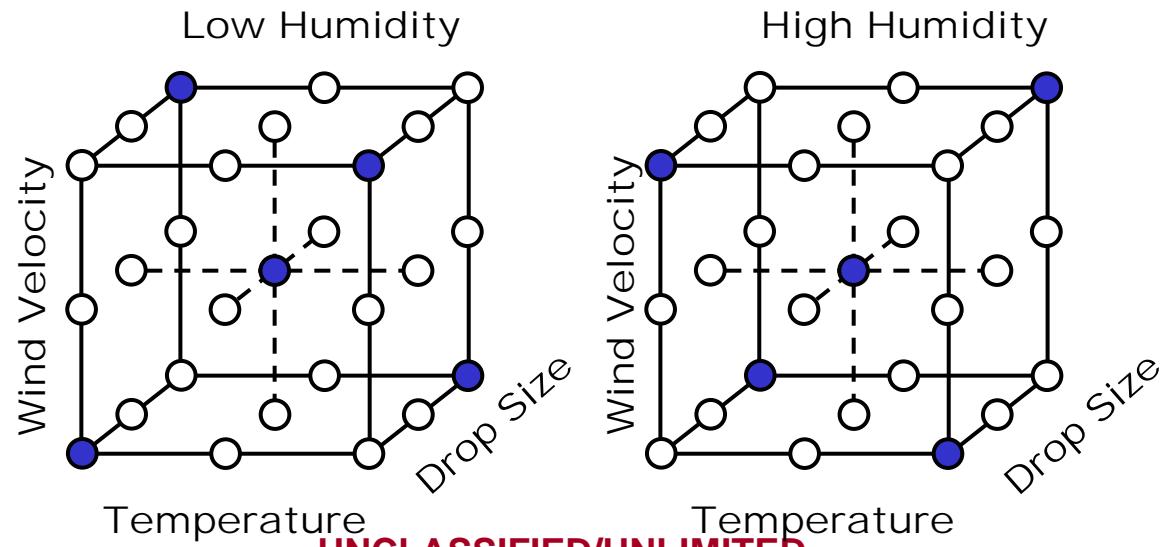
Less than 20% of Originally Planned Trials are Needed to Fit a 5-term Linear Model



Original plan called for running all $3 \times 3 \times 3 \times 2 = 54$ combinations of settings of Wind Velocity (3 levels), Temperature (3 levels), Drop Size (3 levels) and Humidity (2 levels). The 10 blue locations are all that are needed to estimate the main effects which physics-based scaling of the axes showed well-fit the Evaporation Rate data for HD on glass.

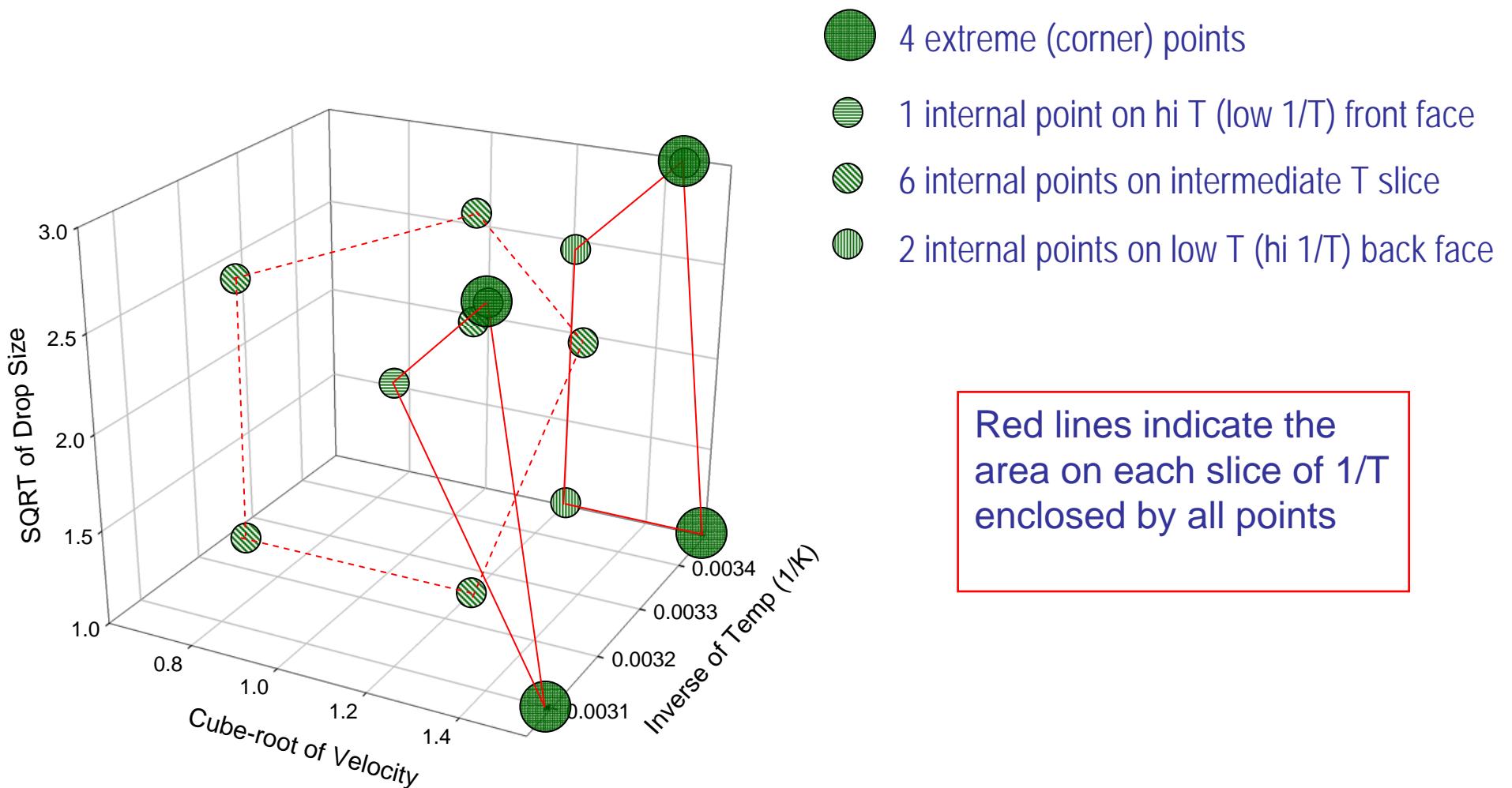
Agents & Substrates other than HD on Glass Will Likely Require More Complex Models

- It still makes sense to acquire data for fitting these models as efficiently as possible.
- Running the trials in randomized blocks of trials will help to facilitate this goal.
- Shown below is a second block that when added to the one on the preceding slide will support the 4 variable 11-term interaction model.





Locations of the 13 Unique Trial Settings for the 10-cm Tunnel

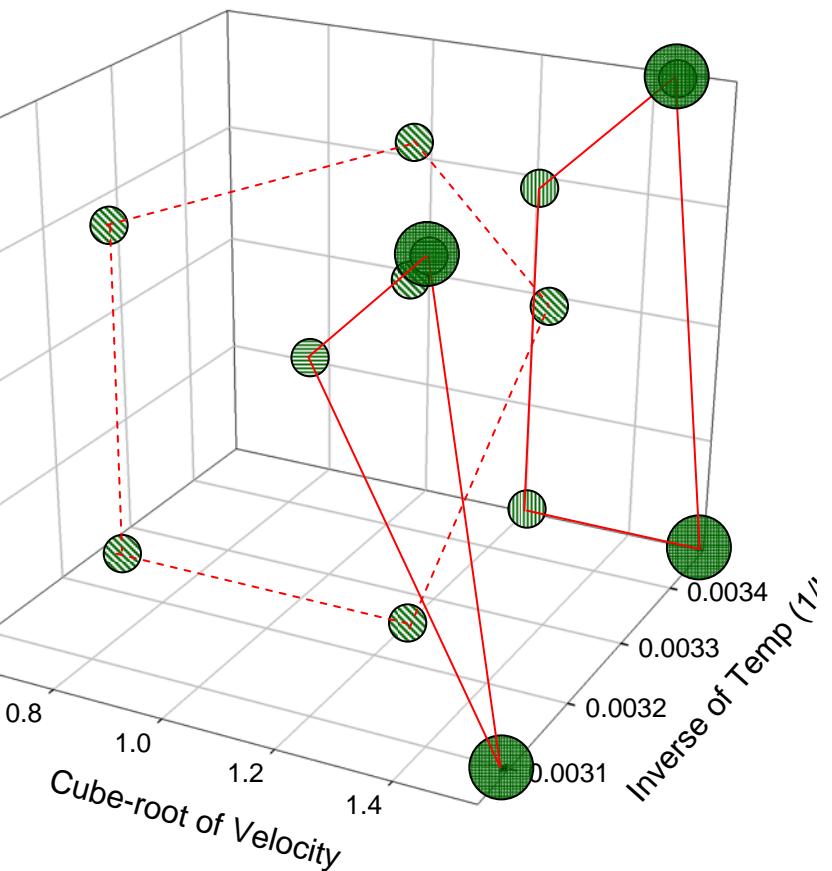
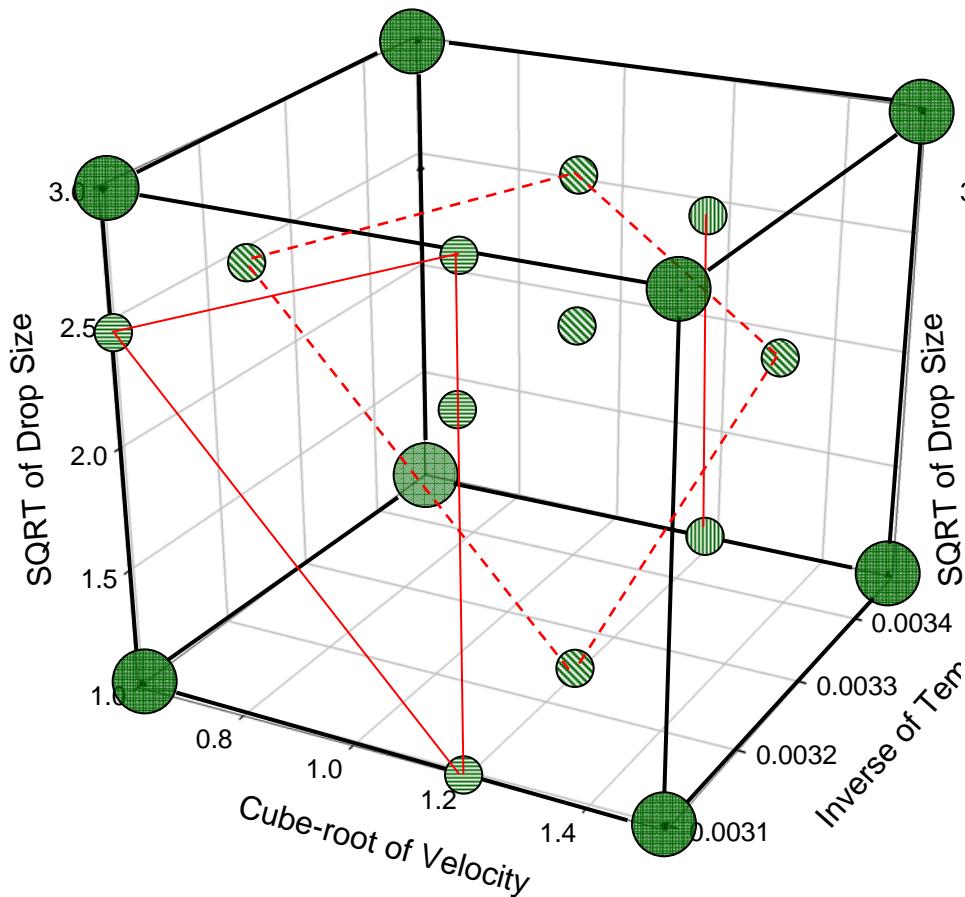




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Locations of the 19 unique trial settings for the 5-cm tunnel

Locations of the 13 unique trial settings for the 10-cm tunnel

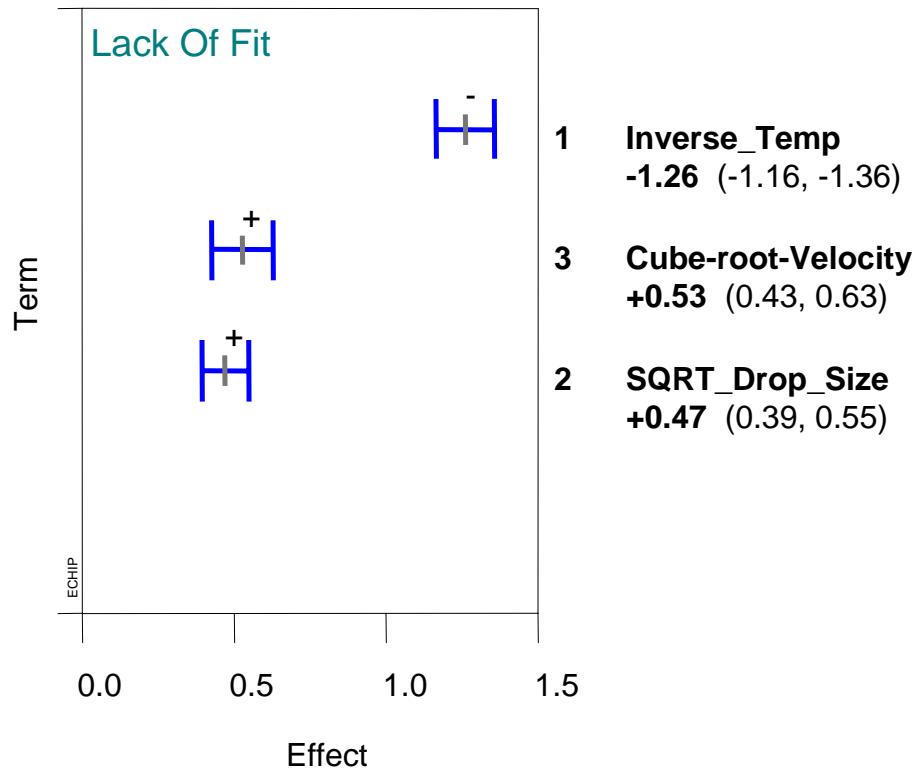


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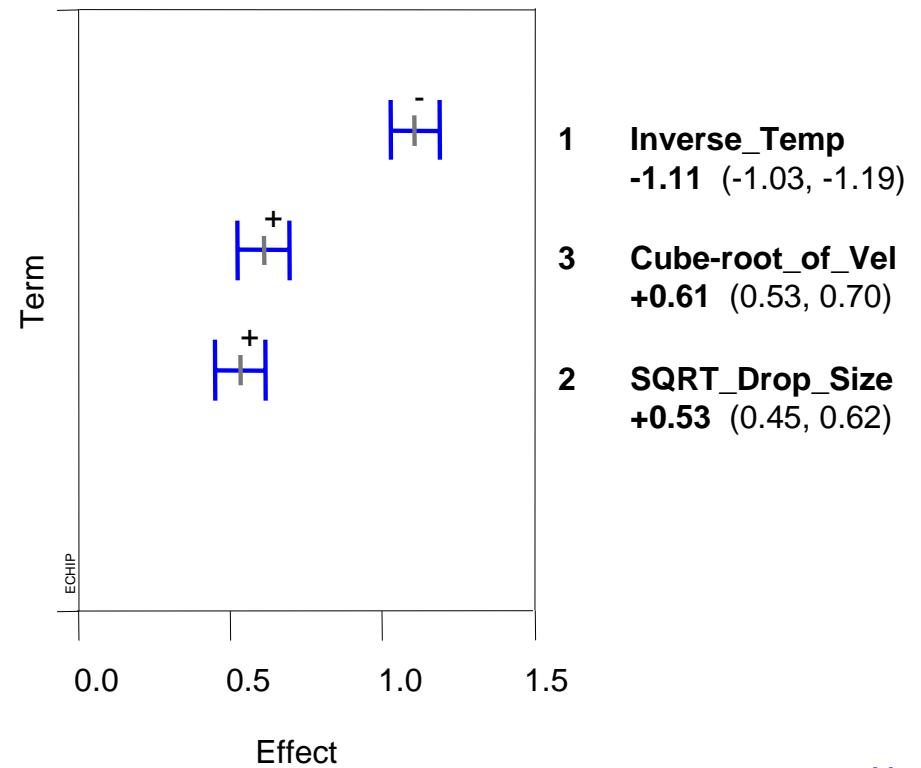
An Effect is the Change in the Response Resulting from Changing a Variable Setting from Low to High

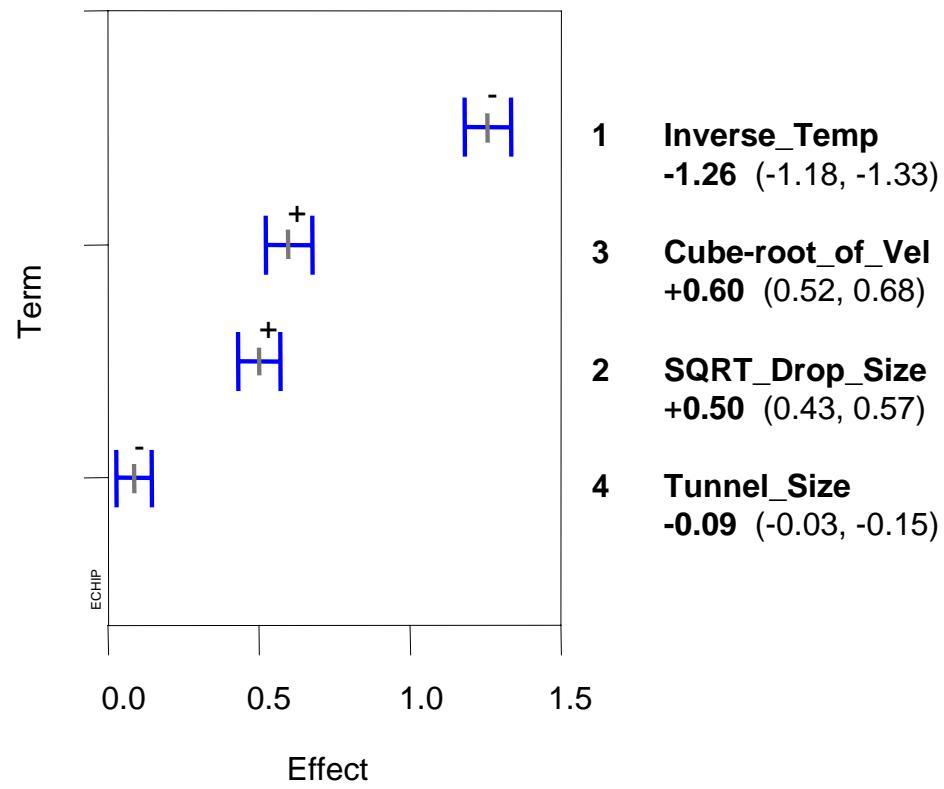
Results for the 2 tunnels are very similar

Pareto Effects for
 $\log_{10}(\text{Evap_Rate})$
10-cm tunnel

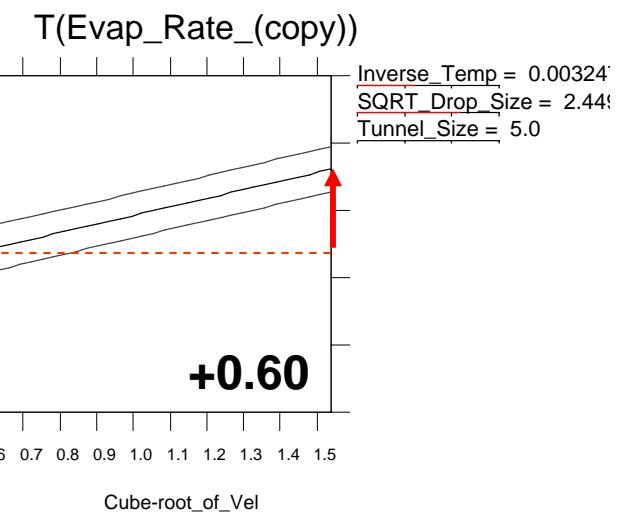
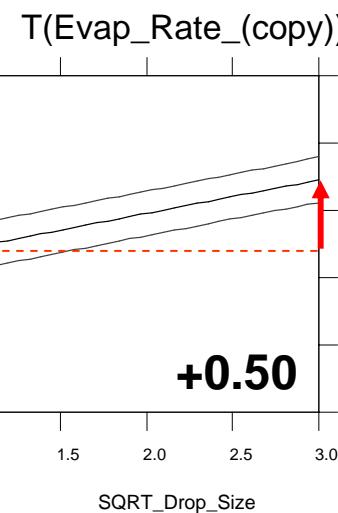
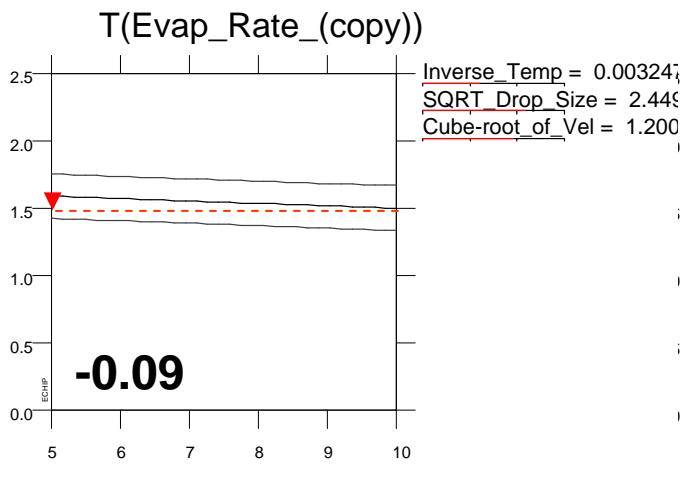
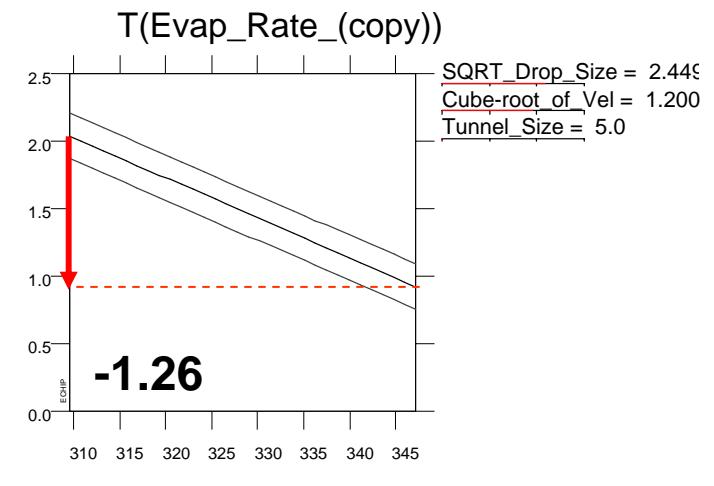


Pareto Effects for
 $\log_{10}(\text{Evap_Rate})$
5-cm tunnel



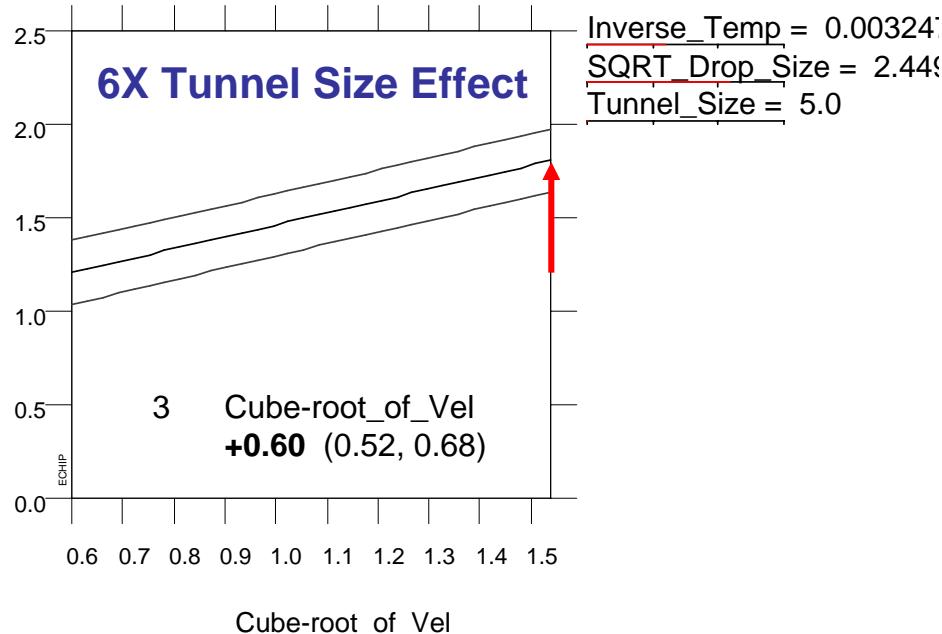


Pareto Effects for
 $\log_{10}(\text{Evap_Rate})$
 including tunnel size
 (5-cm vs. 10-cm)

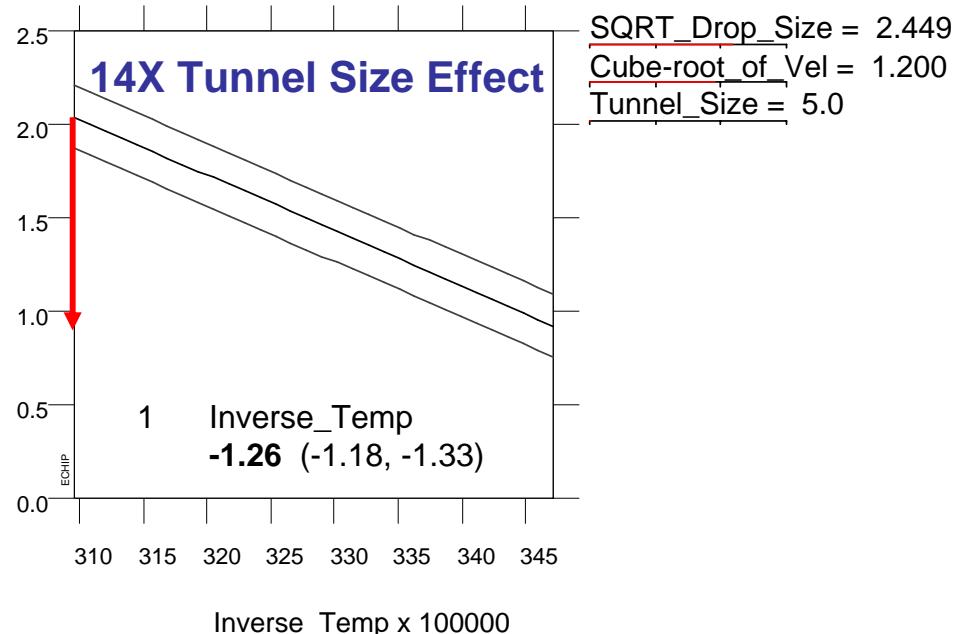


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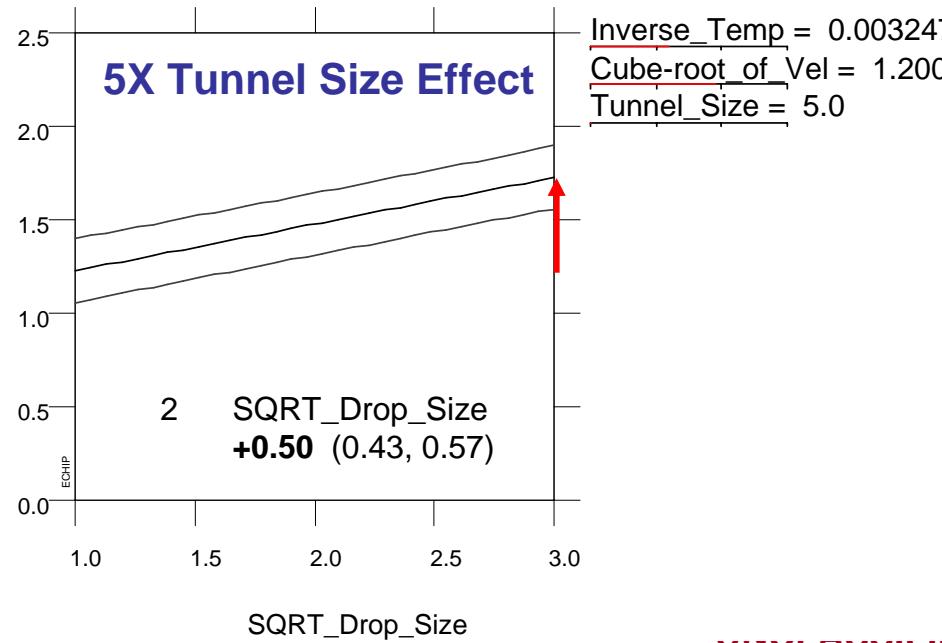
T(Evap_Rate_(copy))



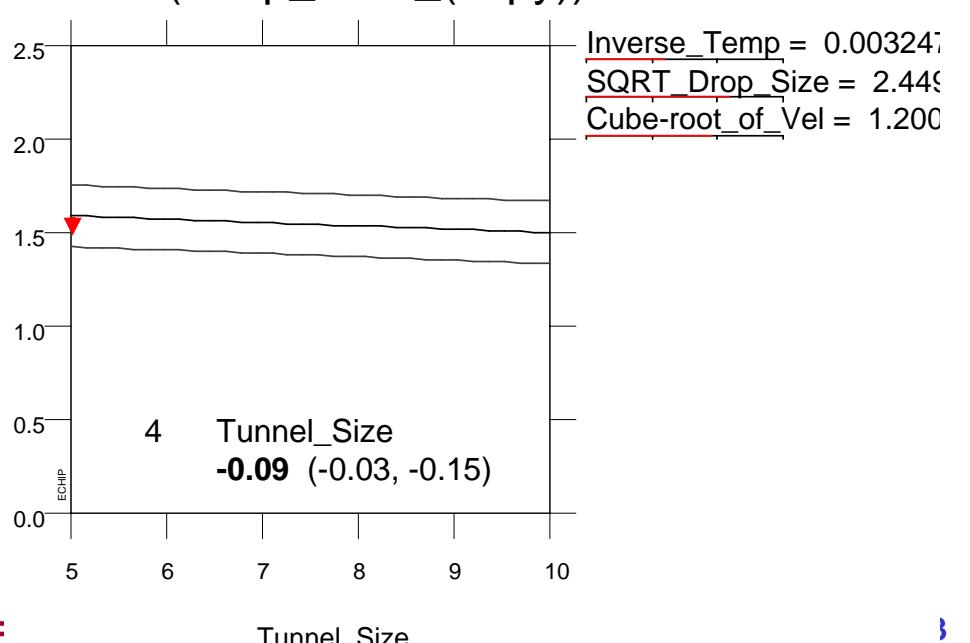
T(Evap_Rate_(copy))



T(Evap_Rate_(copy))



T(Evap_Rate_(copy))





Summary

- Rescaling the variables using knowledge of the physics reduces the complexity of the model required to adequately fit the data
 - Before rescaling, a 10-term quadratic model was needed
 - After rescaling, a 4-term linear model is all that is needed
- Extrapolated predictions for checkpoints within the 5-cm tunnel data validate “nearby” extrapolation with the physics-based linear model
- For the physics-based linear model “farther out” extrapolations are more plausible than those of the empirical model.
 - Note that these conditions are beyond the practical range of the wind tunnels and that these predictions have not been validated.



Summary

- Although the same level of reduction of the number of required trials seen for HD on glass may not hold true for other agents and/or substrates, results point to importance of running trials in a sequence of blocks that support increasingly complex models.
- Combining the data for the 5-cm and 10-cm tunnels shows that the “tunnel effect” - although statistically significant - is dwarfed by the effects of the Temperature, Wind Velocity and Drop Size which are 5X to 14X as large. For HD on glass, the behavior of the two tunnels appears quite similar.